ARMY RESEARCH LABORATORY

BLAKE—A Thermodynamics Code Based on TIGER: Users' Guide to the Revised Program

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Abstract

BLAKE is a general thermodynamics code for use primarily with IBM-compatible desktop personal computers. This code, which was derived from the original version of SRI's TIGER program, is intended primarily for making calculations on the combustion products from conventional military and electrically-heated gun propellants under chamber conditions (temperatures between 1,500 K and 10,000 K, and pressures up to 700 MPa). An important feature of this code is that it embodies a correction for nonideal gas effects appropriate to its primary application. This correction is derived from a truncated virial equation of state in which the second virial coefficient is computed using the spherically symmetric Lennard-Jones 6-12 intermolecular potential. The third virial coefficient is derived from a hard-sphere model.

Another useful feature of the code is that it contains enthalpy data for 60 commonly-used propellant ingredients and some compounded propellants. It also contains enthalpy data for all of the various nitrocelluloses containing from 11.10 to 14.00 percent nitrogen.

This report is a complete guide to the revised code as of December 1997 including some illustrative examples of its use.

Persons desiring a copy of the BLAKE program should address requests to:

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I. INTRODUCTION

The BLAKE computer program is a general equilibrium thermodynamics program derived from an older version of TIGER.[1,2] Although it is applicable to a wide range of chemical equilibrium calculations, BLAKE is specifically intended for computing the properties of gun propellants at chamber conditions. Its principal difference from other chemical equilibrium computer programs is that, like TIGER, it permits the use of several nonideal gaseous equations of state.

The historical background, analysis, and experimental tests of the code are described in an earlier report[3] and will not be repeated here. The present report is exclusively a users' guide.

The original version of the program was run only on main frames but this is rarely the case now. The program BLAKE.EXE described in this report is intended primarily for IBM-compatible computers running under the MS-DOS operating system, or in a DOS window in WINDOWS. With three exceptions the source code itself is written in strict Fortran-77 and so should be easily ported to other computers or operating systems*.

This report specifically describes BLAKE version 221.4. If changes are made in the program after this report has been published, their details will be included as comments in the program's Subroutine VRSION, as will any errors or changes in this report.

II. A NOTE FOR EXPERIENCED USERS

The present version of BLAKE has been little changed from previous versions. The principal changes experienced users should note are these:

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1. BLAKE is based on the original version of TIGER that was developed by Stanford Research International under Contract No. DA-04-200-AMC-3226(X) with the (former) US Army Ballistic Research Laboratories. Dr. Stanley M. Taylor was the Contracting Officer's Technical Representative. This work was documented in an SRI report by Wibenson, W.E., Jr., Zwisler, W.H., Seely, L.B. and Brinkley, S.R., Jr., "Tiger Computer Program Documentation", 1968.

2. A revised and improved version of TIGER is documented in Cowperthwaite, M., and Zwisler, W .H., "Tiger Computer Program Documentation," SRI Publication No. Z106, 1973.

3. Freedman, Eli, *Blake--A Thermodynamics Code Based on Tiger--Users' Guide and Manual*, ARBRL-TR-02411, 1981 [AD A121 259]. An errata list for that report is given in Appendix F of the present report.

* One of the non-standard features is the use of INCLUDE, which, however, is accepted in standard Fortran-90. The other two non-standard features are the use of the Microsft extensions GETDAT and GETTIM, which need to be replaced by the corresponding subroutines specific to the compiler being used. A simple workaround, however, is merely to insert RETURN statements in the five subroutines in the file BLAKETM.FOR.

A. The default unit for enthalpy in the FORmula instruction is now the Joule instead of the calorie. Existing input files with FORmula instructions can still be used, provided the sentinel ',C' is appended to the end of the older instruction. See Sec. V D 15 for details.

B. A PLOt instruction has been added. See Sec. V D 29 for details.

III. THE PROGRAM'S TWO LIBRARIES

A. BLAKE comes with two libraries, a 'standard' one for use with temperatures in the range 300 - 6000 K, and an 'extended' one for use with temperatures in the range 3000 - 10000 K.[4] The names of the alphanumeric files containing them are SBLAKLYB.LIB and XBLAKLYB.LIB, respectively. The data in these libraries have been completely refitted for this report.

B. The program does not use these libraries directly; they are used in binary forms produced by an auxiliary program, FRMLIB (see Sec. VII). The corresponding binary forms are named SBLAKLYB.DAT and XBLAKLYB.DAT , respectively. Copies of all of these libraries (alphanumeric and binary) are included on the distribution disk.

C. A user who makes any change to the data in either alphanumeric library must then recreate the corresponding binary library with FRMLIB.EXE.

D. The program always starts with SBLAKLYB.DAT but can be switched to the other library by an instruction (see LIBRARY in Sec. V D 22).

IV. SCOPE OF THE LIBRARIES

A. The Standard Library.

1. *Elements*. The standard library contains data for compounds of the 21 elements listed in Table 1.

Table 1. The Elements Included in the BLAKE Library

Aluminum	Chlorine	Hydrogen	Magnesium	Sodium
Argon	Electron	Iron	Nitrogen	Sulfur
Barium	Fluorine	Lead	Oxygen	Titanium
Boron	Helium	Lithium	Potassium	Zirconium
Carbon				

---

4. The development of the extended library is discussed in detail in Oberle, W.F. and Freedman, Eli, "Preparation and Extension of the Thermodynamics Program BLAKE and Its Library to 10,000 K for Use with Electrothermal-Chemical (ETC) Systems," ARL-TR-488 (July 1994). The rationale for excluding charged species is presented here.

2. *Gaseous Species.* The 88 neutral gaseous species listed in Table 2 are possible products in every BLAKE calculation (provided the requisite elements are present).

Table 2. The Gaseous Species Included in the BLAKE Library

Al_2O	CH_2	FeO_2H_2	K_2F_2	NH_3
AlF_2O	CH_2O	Formic acid	$K_2H_2O_2$	NO
$AlHO_2$	CH_2OH	H	KBO_2	NO_2
AlO_2	CH_3	H_2	Ketene	NS
Argon	CH_3Cl	H_2O	KH	O
B_2O_2	CH_3CN	H_2O_2	KO	O_2
B_2O_3	CH_4	H_2S	KOH	OH
$B_3H_3O_3$	CH_4O	HAlO	MgO_2H_2	Pb
BaO_2H_2	CHO	HCl	N	PbS
BH_2	Cl	HCN	N_2	S
BH_3	CN	Helium	N_2O	S_2
BHO	CO	HF	NaF	S_2O
BHO_2	CO_2	HNCO	NaOH	SH
BO	COS	HNO	NCO	SO
C	CS	HNO_2	NH	SO_2
C_2H_2	CS_2	HO_2	NH_2	TiO_2
C_2H_3N	Electron	K	NH_2OH	ZrO
C_2H_4	$FeCL_2$	K_2		

Up to 56 of these gaseous species may be present in any one computation.

In addition to these species, thermodynamic data for 8 more species, which are listed in Table 3, are furnished. Before they can be used, a user must first remove the initial 3 blanks in front of CON (see Sec. VII C 1), and then reform the binary library with FRMLIB.

Table 3. Gaseous Species for Which Thermodynamic Data Are Furnished, But Which Must First Be Processed By a User

CH_2OH	CH_4O	HO_2	NCO
CH_3CN	H_2O_2	Ketene	NH_2OH

3. *Condensed Species.* The program library contains data for 16 species in condensed phases that are listed in Table 4.

Table 4. The Condensed Species Included in the BLAKE Library

Species	Phase(s)	Species	Phase(s)
Al_2O_3	solid and liquid	KOH	liquid only
B	solid and liquid	K_2S	solid and liquid
B_2O_3	solid and liquid	MgO	solid and liquid
BC_4	solid only	NaF	liquid only
BN	solid only	Pb	solid and liquid
C(s)	solid only	Ti_4O_7	liquid only
KF	liquid only	TiO_2	solid only
K_2CO_3	solid and liquid	ZrO_2	solid and liquid

B. The Extended Library.

1. *Elements.* The extended library contains data only for argon, helium, compounds of C, H, N , and O, and the electron.

2. *Gaseous Species.*

a. The extended library contains data for the 29 species listed in Table 5.

Table 5. The Species in the Extended Library.

Ar	CCORA*	CO_2	HCO	NH_2
C	CH	Electron	He	NO
C_2	CH_2	H	HO_2	O
C_2H	CH_3	H_2	N	O_2
C_2H_2	CH_4	H_2O	N_2	OH
C_2H_4	CO	HCN	NH	

*CCO radical

b. In addition, thermodynamic data for two species, $H_2C{=}C$ and O_3, are in the alphanumeric library but not in the binary library; they may be added to the latter at any time by users who so wish.

c. Notice that there are no ionic species in Table 5 (other than electron). The justification for this omission is presented in Ref. 4.

3. *Condensed Species.* There are no condensed species in the extended library.

V. THE INSTRUCTION SET FOR BLAKE

A. General Remarks.

1. BLAKE, following TIGER, proceeds by executing one by one a series of instructions.

2. The source code has room for 70 instructions of which 43 are used. In fact, only two instructions (COMposition and GUN) suffice for BLAKE's primary application, the computation of the adiabatic flame temperature. Adding two more (POInt and ISOline) permits the computation of a constant-breech pressure gun simulation.[5]

a. Since the *Users' Guide* (Ref. 1) was first published, some new instructions have been added and some old ones (CoMmenT, DATe, ECHo, and TRAnsport) have been made effectively inert; the program ignores them but does not abort if they are entered as it does for an unrecognized instruction.

b. The instruction STArt [of library] has been superseded by the program FRMLIB (which is also on the distribution disk); a note to this effect is printed if this instruction is used.

c. As each instruction is encountered by the program, it is echoed to the output file.

d. Table 6 gives the complete list of all instructions with very brief descriptions.

B. There is no prescribed rigid order for instructions other than the order required by logic. For example, no computation can be executed until a valid COMposition instruction has been entered.

1. Each instruction consists of a key word or abbreviation followed by a variable number of fields containing keywords or numbers. Each field is set off from its neighbors by commas. The keyword or abbreviation for the instruction itself must appear in columns 1-3 of the instruction; otherwise the fields are arbitrary in both length and placement in the line.

2. Letters may be entered in either UPPER CASE or lower case. The program uniformly converts them to upper case, except for titles which are left as typed.

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5. Kotlar, A.J., "The Effect of Variable Composition Equilibrium Thermochemistry in Constant Breech Pressure (CBP) Gun Simulations," *Ballistics '95: 15th International Symposium on Ballistics (Proceedings)*, IB16, Vol. 3, pp 119-126; 1995.

Table 6. The BLAKE Instruction Set

Column headings:

A: A running number; it corresponds to those used in Sec. V D.

B: The instruction's 3-character abbreviation. These 3 characters must be used and must be in cols 1-3; additional following characters are ignored until a comma occurs.

C: The actual instruction number in the source code.

D: A brief description; complete details are given in Sec. V D.

A	B	C	D
1.	BOM	30	Closed-bomb calculation
2.	BPR	29	Toggles virial coefficent print
3.	CHO	6	Chooses product gases
4.	CM2	11	Composition-2 (2-line composition)
5.	CMT	30	Comment (ignored)
6.	COM	29	Composition
7.	DAT	6	Date (ignored)
8.	DEB	11	Debug
9.	DEL	28	Sets temperature step for virials
10.	DES	9	Destroy
11.	ECH	53	Echo (ignored)
12.	EXG	51	Constant volume gas explosion
13.	EXP	44	Isochoric explosion
14.	FLO	7	Floor
15.	FOR	3	Formula
16.	FRE	15	Freeze
17.	GEO	13	Selects gaseous equation of state
18.	GRI	46	Grid
19.	GUN	50	Executes gun chamber calculation
20.	ING	55	Obtains input from external file
21.	ISO	45	Isoline
22.	LIB	34	Interchanges libraries
23.	LJP	26	Sets L-J Parameters
24.	MEL	16	Melt
25.	MOR	31	Controls output from GUN
26.	MUL	54	Changes multiplier for third virial
27.	ORC	19	Order condensed species
28.	ORD	5	Order
29.	PLO	14	Prepares ASCII tables for plotting
30.	POI	41	Point instruction
31.	PRL	1	Print limiter
32.	QEX	8	Heat of explosion
33.	QUI	3	Quit (same as Stop)
34.	REC	48	Recall results
35.	REJ	4	Reject
36.	RET	8	Retain
37.	SAV	7	Save results for reuse
38.	STA	1	Start of library (ignored in BLAKE)
39.	STO	9	Stop. Same as QUIt
40.	TIM	4	Timer
41.	TIT	2	Title
42.	TRA	?	Transport properties (ignored)
43.	UNI	5	Units

3. When numbers are required in an instruction, they may be typed in free form. Example: 69, 69., 69.0, 0.69E2, and 0.0069E04 all represent the same number in an instruction. The program decides eventually whether it needs a real number or an integer and takes appropriate action.

C. The general form of an instruction is

INStruction, PAR1, <n1>, PAR2, <n2>, PAR3, <n3>, ..., [PARm, <nm>]
or
INStruction, <a1>, <b1>, <a2>, <b2>, <a3>, <b3>, ..., [<an>, <bn>]

or combinations of these forms.

1. Names or letters printed in the descriptions in CAPITALS are KEYWORDS and must be spelled just that way, except that as noted previously, a user may enter them in either upper or lower case; no other variation is permitted. Additional letters are added to the name of some of the instructions for mnemonic reasons but are not part of the name and may be omitted. Example: FOR, FORmula, and FORmulas are interpreted as the same instruction and are all valid.

2. Quantities printed in lower-case letters in the definition of an instruction represent numbers that must be entered. Names of quantities enclosed in angle brackets (< >) indicate the name of the quantity for which a number must be entered.

3. Commas mark the end of each field and separate succeeding fields from each other. They must be used exactly as noted. In some cases, double commas with at most blanks between them have a special significance; their use is explained in the appropriate instructions.

4. The ellipsis, ..., indicates that a variable number of items may be entered.

5. Items in square brackets are optional as noted for individual instructions.

6. The vertical stroke, |, indicates that one or another of the items separated by it may be chosen, but not both. Example:

ISO, P | T, ...

means that the key letter P or T may be used, but not both at the same time.

7. The instructions are listed in alphabetic order by their three-letter key.

8. Examples of the outputs produced by the computational instructions are given in Sec. IX.

D. The Details of Each Instruction.

1. BOMB

Forms: BOMb, V, <vol of bomb>, W, <mass of sample>
or
BOMb, W, <mass of sample>, V, <vol of bomb>.

Description: This instruction computes the thermodynamic state reached when a sample of mass W is completely burned in a closed bomb of volume V.

Example:

BOM, V, 875, w, 37

2. BPRINT

Form: BPRint

or
BPRint, <number>

Description: This instruction tuurns on or off the printing of the virial coefficients of the composition being computed. When it is 'on', a file named VIRIALS is opened and three lines of output are added to it for each succeeding computation.

The default setting is 'off'.The instruction BPR is a toggle; if it had been 'off',it is set to 'on', and *vice-versa*. Each new run deletes the previously existing file (if any). Whenever it is 'on',entries accumulate throughout the run.

Example: BPR

3. CHOOSE

Form: CHOose, <name1>, <name2>, <name3>, ...

Description: This instruction forces the program to consider only the named constituents as possible products of an equilibrium calculation. The names listed must be constituent names in the library. The use of this instruction is recommended only in special cases; for example, if the user wants to restrict the equilibrium products to only CO, CO_2, H_2O, H_2, and N_2, using the CHOose instruction would be the easiest way to accomplish it.

Example:

CHO, CO_2, H_2O, N_2, CO, NH_3

4. CM2 [COMPOSITION2]

See the discussion under COMposition (instruction 6).

5. CMT [COMMENT]

Description: This instruction is no longer active; if used, it is silently ignored.

6. COMPOSITION

Form: COMposition, <name1>, <a1>, <name2>, <a2>, <name3>, <a3>, ... [,MOLE]

Description: This instruction defines the composition of a mixture. It is an essential instruction, as any computational instruction is automatically rejected if it occurs before a COM instruction.

The names <name1>, <name2>, ..., must have previously been defined by FORmula instructions; if not, the entire instruction is rejected. The quantities <a1>, <a2>, ..., are the relative amounts of each substance. The order of the names is immaterial, but the correct amount must follow each name. The amounts need not be percentages; any basis is acceptable. Regardless of how the composition is entered, however, the program will normalize it and print the results as both weight percent and mole percent.

If the keyword MOLE is entered, then the composition data must be in moles but not necessarily in mole percents.

All of the data must fit into one 80-column line. If this is not feasible, use the instruction CM2 instead of COM. The user may then extend the input data over two 80-column lines. Do not repeat CM2 at the start of the second line. The MOLE designator does not apply to CM2.

Examples:

```
COM, NC1325, 75, NG, 25
COMPOS, N2, 4, O2, 1, MOLE
CM2, nc1325, 72, dbp, 18,
        ng, 6, c, 0.2, h2o, 0.3
```

7. DATE

Description: This instruction is no longer active; if used, it is silently ignored.

8. DEBUG

Form: DEBug, <n>

Description: If <n> is not 0, the debug feature is turned on; if zero, it is turned off.

This instruction was taken over from TIGER where it was introduced for assistance in developing Subroutine ECOMPO. When turned on it prints the current temperature, pressure, volume, entropy, and energy on each pass through Subroutine ECOMPO.

Originally it also printed the current mole numbers and the current corrections to the mole numbers on each pass, but this output has been commented out. Overall this feature has not proved to be useful with BLAKE.

Example: Deb, 1

9. DELTEM

Form: DELtem, n

Description: Second virial coefficients are not strong functions of temperature in the range of flame temperatures, so there is no need to recompute them for every small change in temperature. They are recomputed when the change is greater than DELTEM. Its default value is 0.5.

This instruction changes the value to n provided n is greater than zero; if zero or a negative value is entered, it is ignored.

Example: DEL, 2

10. DESTROY

Form: DEStroy

Description: This instruction negates the effect of a RETain instruction (see instruction 36).

Example: DES

11. ECHO

Description: This instruction has been superseded; if used, it is silently ignored. *All* BLAKE instructions are echoed to the output file.

12. EXPLOSION, GASEOUS

Forms: EXG, P, <p>, T, <t> [, MM]

or

EXG, T, <t>, P, <p> [, MM]

Description: This instruction is almost the same as EXP (instruction 13) except that it is for a gaseous mixture at pressure <p> and temperature <t>. The ideal gas law is used to calculate the volume and then EXP is called automatically. The initial energy cannot be changed.

The input pressure must be in megapascals unless the sentinel MM is present, in which case the input must be in Torricelli (millimeters of mercury).

Example: EXG, P, 2, T, 298.15

13. EXPLOSION [Constant volume condensed phase]

Form: EXPlosion, V, <vol> [, EOF, <u>]

Description: This instruction executes a constant-volume (isochoric) burning calculation on a previously-defined mixture. The specific volume, <vol>, is in cubic centimeters per gram unless the user has changed the volume conversion factor. Normally the energy of formation calculated for the composition is used; if the user wants to use a different one, enter the key symbol EOF and the specific energy <u>.

Example: EXP, V, 5

14. FLOOR

Form: FLOor, <n>

Description: This instruction sets the level of the floor at <n>. See the discussion in Appendix A on TIGER's computation of equilibrium. In a case where a user is having a lot of trouble forcing a particular computation to converge, it sometimes helps to 'raise' the floor; *i.e.*,make <n> a smaller number than the program value; sometimes it doesn't help. Once a new floor has been set, it remains at that value until either a new COM or a new FLO instruction is entered.

Example: FLO, 11

15. FORMULA

Form: FORmula, <name>, <enth>, <ele1>, <n1>, <ele2>, <n2>, <ele3>, <n3>, ..., [C | c]

Description: This instruction defines <name> as the name of a reactant species; its enthalpy or energy of formation is <enth> and its formula contains <n1> atoms of element <ele1>, <n2> atoms of <ele2>, ...,. The symbols used for the elements must be exactly those that appeared in an ELEment instruction when the library was formed (see Sec. VII C 2).

Depending on the particular computation to be performed, the input energy in a FORmula instruction may be the enthalpy or the energy of the substance. This point is discussed in Appendix C. The enthalpy of formation is entered in Joules per gram-mole, not Joules per 100 grams, and not kilojoules per mole. If, however, the sentinel C or c is entered, then the enthalpy must be entered in calories per mole.

Note that enthalpies must be in Joules. Nevertheless, existing FORmula instructions containing enthalpies in calories may still be used if the sentinel ,C or ,c is appended to the instruction.

In keeping with the TIGER and BLAKE convention for putting numbers in instructions, the numbers <n1>, <n2>, ..., may be typed in any way. The program uses them as real numbers so decimal fractions are accepted and used correctly. When the program prints the formula, however, these numbers are converted to integer form by truncation, not rounding, so that decimal fractions will not be printed properly although the program uses them correctly.

This gives the appearance of trouble with polymers whose formulas rarely contain integral numbers of atoms. Customarily polymer compositions are specified in units such as gram-atoms per hundred grams with a corresponding enthalpy; BLAKE, however, does not accept such input data. They are easily converted to molecular formulas, but the numbers of atoms generally come out to be decimal fractions. This creates a small but annoying problem, since one usually prefers to have the correct formulas printed for the input. The simplest solution is to multiply the formulas and the associated enthalpy by 100, 1000, 10000, or whatever multiplier is needed.

The formulas of many common propellant ingredients are prestored in the program and need not be entered in a FORmula instruction. The names, heats of formation, molecular weights, and formulas of these substances are listed in Appendix C.

If a FORmula instruction with a duplicate name is entered, a warning message is printed, and the data from that instruction replaces the previously stored data. *Note that this is a change from previous versions, which rejected the duplicate instruction.*

The program does some checking on FORmula instructions. If an error is found, the instruction is rejected and an error message is printed. A maximum of 50 additional formulas is permitted; if the user tries to enter more, they are rejected and an error message is printed.

Examples:

```
FORM, DBS, -280E3, C, 18, H, 34, O, 4
FOR, Pg, -4E7, c, 4000, h, 5000, o, 100
```

16. FREEZE

Form: FREeze

Description: Almost all BLAKE calculations are carried out with the assumption of total dynamic chemical equilibrium. The FREeze instruction inhibits ('freezes') all chemistry so that all subsequent calculations are done on a mixture of non-reacting gases. Unfortunately this instruction does not always work properly; see the discussion for the ISOline instruction (instruction 21 below). A FREeze instruction remains in effect until ended by a MELt (instruction 24 below).

Example: Freeze

17. GEO [GASEOUS EQUATION OF STATE]

Form: GEO, [IDEAL | VIRIAL | LJ]

Description: Change the Gaseous Equation Of state to either of the following:

Keyword	Equation of State
IDEAL	Ideal
VIRIAL or LJ	Truncated virial

The default equation is the truncated virial equation. If the KEYWORD is mistyped, the program defaults to the truncated virial. Earlier versions of BLAKE also had the BKW and NBS (Powell-Wilson-Haar-Klein) equations of state. The former is not useful for ballistic calculations, and the latter, for unknown reasons, did not work properly in BLAKE. The coding for both equations has been left in Subroutine NONIDL, but neither can be accessed by the GEO instruction. The user who wants to try either one will have to make some programming changes and then recompile.

Example: Geo, ideal

18. GRID

Forms: GRId, CENTER, P, <ip>, <np>, <fp>, V, <v1>, <nv>, <v2>
or
GRId, CORNER, P, <p1>, <ip>, <p2>, V, <v1>, <iv>, <v2>

Description: This instruction computes chemical equilibrium at a grid of points centered about, or cornered at, a specific point. The computations may be done only for the following combinations of thermodynamic variables:

pressure and volume (P, V);
pressure and entropy (P, S);
volume and temperature (V, T);
volume and energy (V, U); and
volume and entropy (V, S).

In each of these cases, the parenthesized letters are the key letters that must be used in the instruction. In all cases the order must be exactly as listed here.

The units for the various quantities must be the program's default ones: megapascals, Joules, and cubic centimeters for pressure, energy, and volume, respectively. The units of the extensive variables (enthalpy, energy, volume, and entropy) are specific; that is, for one gram of substance.

<p1> is the initial value of the variable (P, in this case); <p2> is its final value. For CORNER, <ip> and <iv> are the *sizes* of the increments in those variables. For CENTER, <np> and <nv> are the *number* of increments to be inserted between initial and final values. The increments <ip> and <iv> may be negative if desired.

If instead of a number, a comma with no intervening characters other than blanks is used, the program will automatically use the existing value of that variable.

Examples: GRID, CORNER, P, 1, 0.1, 10, V, 20, .5, 40
GRID, CENTER, P, 1, 4, 10, V, 20, 19, 40
gri, center, p, , 4, 10, v, , 19, 100

19. GUN

Form: GUN, <s>, <i>, <f> [, <u>]

Description: This instruction is a special case of the EXPlosion instruction with its output designed for ballistics. It computes the thermodynamic properties of the chamber gas produced by a propellant burning to equilibrium at constant volume. The starting loading density is <s>; it is incremented by amounts <i> up to the final value <f>. A maximum of 32 different loading densities is permitted by a single GUN instruction. If a user tries to use more than 32, only the first 32 are computed and the program continues to the next instruction.

<u> is an optional number; it represents added energy in kilojoules per gram of mixture. This feature is useful for electrothermal gun computations. <u> must be a number; otherwise the instruction will be rejected.

Examples: GUN, 0.05, .05
Gun, 0.01, .01, .2, 5

20. INGREDIENT

Form: INGredient

Description: This instruction makes the program read data on formulas from a separate file that must be named INGREDS.DAT and stored in the same directory. A file with this name is furnished with the distribution disk; a user can delete or add to it, subject to the limit of 49 additional FORmulas.

Example: Ing

21. ISOLINE

Form: ISOline, <VarF>, <vf>, <Varl>, <p1>, <np>, <p2> [, LOG]

Description: This instruction computes thermodynamic equilibrium for a set of points of which the first variable is held constant while the second one is incremented. The fixed

thermodynamic variable is <VarF>; its value is <vf>. The thermodynamic variable to be incremented is <Varl>; its initial value is <p1>; <np> is the *number* of increments; and <p2> is the final value of the variable. <p1> may be less than or greater than <p2>.

If the optional keyword LOG appears, logarithmic spacing is used. Logarithmic spacing is automatically used when the variables are (S, V).

If two successive commas with at most blanks between them appear in place of <vf>, the program uses the existing value.

Only 7 pairs of variables may be used, but either variable of a pair may be the fixed one or the incremented one. The 7 pairs are

P, T or T, P
P, H or H, P
P, S or S, P
P, V or V, P
V, T or T, V
V, U or U, V
V, S or S, V

One might expect that any ISOline instruction that entails cooling or expansion ought to work in conjunction with a FREeze instruction, but this is unhappily not the case.* In particular, frozen isentropic calculations do not work. Kotlar [6] has used a combination of BLAKE instructions to work around this problem. For example, to evaluate the frozen calculation, ISO, S, 9.012 , V, 5, 5, 100, which does not work, he ran a series of frozen ISO, V, 100, T, ... calculations that eventually closed in on the triplet (S, V, T) = (9.012, 100., 1774).

Examples: ISO, T, 1000, P, 10, 4, 20
ISO, S, , V, 5, 7, 100
Iso, P, 2000, V, 5, 7, 500

---

* The reason for the failure of some ISOline instructions to work when frozen is unknown. Later versions of TIGER do not have this difficulty.

6. Kotlar, A.J., US Army Research Laboratory. Private communication to Eli Freedman, June 1995. This technique is used implicitly in his paper, Kotlar, A.J. "The Thermodynamics of Interior Ballistics and Propellant Performance" *Proceedings, 29th JANNAF Combustion Conference*, CPIA Publication 593 (October 1992). In reading this paper, the designations *static* and *dynamic* are used for *freeze* and *melt*. This must be kept in mind in order to read the tables correctly.

22. LIBRARY

Form: LIB

Description: The instruction LIB is a toggle; it changes whatever library is in use to the other one. When the program is first started, the standard library (see Sec. III) is the one in use.

Care should be taken to switch libraries only before a COM instruction. The program does not check whether the LIB instruction has been entered appropriately or not. If, for example, it is entered just before a GUN instruction, the ensuing results will be incorrect.

Also, the extended library contains only compounds of C, H, N, and O; therefore, unpredictable results may be expected if calculations using this library are attempted on compositions containing additional elements.

Example: LIB

23. LJP [Change Lennard-Jones Parameters]

Form: LJP, <name1>, T | E, <v1>, S | D, <v2>, <name2>, T,<v3>, S, <v4>, ...

Description: This instruction changes the values of the Lennard-Jones parameters for substances <name1>, <name2>, ...,. Each <name*i*> must appear in the library as a constituent. The program checks that both parameters have been entered, even if the user only wants to change one of them. Changing only one is simplified by the fact that if two successive commas with at most blanks between them appear in place of <v1> (or <v2>, ...) the program uses the existing value.

The order of T and S is immaterial, but <v1> and <v2> must correspond to the key letters used. The key letter T may be replaced by E; and S, by D.

If <name1> is mistyped or is an illegal name, no action is taken but a diagnostic message is printed. If two or more names appear in an instruction and one of them is wrong, the program will nevertheless attempt to process the remaining names.

If no COMposition instruction has been entered, the program will reject any LJP instruction. A suitable message is printed.

Examples: LJP, H2O, T, 600, D, ,
LJP, NH3, D, 4, T, 350

24. MELT

Form: MELt

Description: This instruction undoes the effect of a FREeze instruction.

Example: Mel

25. MORE

Form: MORe, <n>

Description: When <n> is non-zero, this instruction produces additional output for the GUN instruction. See case 2 in Sec. IX for details.

Example: MOR, 1

26. MULTIPLIER

Form: MULtiplier, <n>

Description: The third virial coefficient of molecule i in BLAKE is computed by the equation

$$CVIRL(i) = XMUL * 0.1765 * [1.26135 * SIG(i)^3]^2$$

where SIG(i) is the Lennard-Jones diameter of the molecule. Hirschfelder *et al.*[7] give the details of the computation of the second and third virial coefficients using Lennard-Jones' formalism.

XMUL is a multiplicative factor whose default value is 1.0. This instruction permits a user to change the factor to any other value, <n>. Once MULtiplier has been used, XMUL retains its value even after a new COMposition has been entered. Furthermore, a succession of MULtiplier instructions, without new COMposition instructions, will probably not work. The reason for this is that MULtiplier is only effective when a new set of virial coefficients is computed, but the program does this only when two successive temperatures differ by at least 0.5 K (see DELtem, instruction 9). Thus, a sequence of pairs of GUN and MULtiplier instructions without intervening COMposition instructions is unlikely to give correct answers.

Example: MUL, 0.11

---

7. Hirschfelder, J.O., C.F. Curtiss, and R.B. Bird, *Molecular Theory of Fluids*, John Wiley & Sons, New York (1954), Chap. 3.

27. ORC [ORder Condensed Constituents]

Form: ORC, <name1>, <name2>, <name3>, ...

Description: This instruction is very similar to the ORDer instruction (see instruction 28 below), except that ORC applies only to condensed constituents, whereas ORD applies only to gaseous ones. <name1>, ..., must be the names of existing product species. If they are not, an error message is printed and the program skips to the next case.

ORC is not often needed, but in some cases (*e.g.*, black powder--see Cases 3a-3c in Sec. IX) it is necessary.

Example: ORC, K2SO4$

Note: A formula ending in '$' means that that species occurs in a condensed phase (solid or liquid or both). The formula for graphite, however, is C(s).

28. ORDER

Form: ORDer, <name1>, <name2>, <name3>, ...

Description: This instruction makes the program choose <name 1>, <name2>, ..., as the components for the first attempt at finding the equilibrium composition. (See the discussion in Appendix A on the way TIGER works.) If these components are not all linearly independent, one or more of them will be omitted. The names of the constituents must be exactly the same as the names used in the CONstituent instruction when the binary library was formed (see Sec. VII C 1). Also, none of these substances may have been previously rejected by a REJect instruction (see instruction 35 below). If either of these conditions is violated, a warning message is printed and the program aborts.

Example: ORD, N2, H2O, CO2

29. PLOT

Form: PLOt

Description: When this instruction is activated, the GUN instruction creates an ASCII file named BLAKE.PLT containing the loading density, the weight-per cent amounts of the ingredients up to a maximum of five, and the following equilibrium thermodynamic properties: temperature, pressure, impetus, molecular weight, co-volume, frozen gamma, ballergy, and internal energy.

The instruction PLOt is a toggle; if it had been 'off', it is now 'on', and *vice-versa*. Its initial (default) setting is 'off'.

BLAKE.PLT is recreated with each new run that contains a PLOt instruction. If, in the course of a run, a user toggles PLOt on and off, BLAKE.PLT accumulates the data during

the 'on' cycles. Once the file BLAKE.PLT is created, it remains in the directory indefinitely until the user deletes it.

Example: PLO

30. POINT

Forms:
POInt, P, <p>, T, <t>
or
POInt, P, <p>, V, <v>
or
POInt, P, <p>, H, <h>
or
POInt, V, <v>, U, <u>
or
POInt, V, <v>, T, <t>
or
POInt, V, <v>, S, <s>

Description: This instruction computes chemical equilibrium at a point with a specified pair of thermodynamic variables. The possible variables are pressure (P), volume (V), temperature (T), enthalpy (H), internal energy (U), and entropy (S).

In each case the upper case letter denotes the variable; and the lower case letter denotes its value in the established units (see Sec. VI C 1). The quantities volume, enthalpy, internal energy, and entropy are intensive; that is, for one gram of mixture.

Only the listed orders are accepted. For example, the instruction POI, T, <t>, P, <p> is unacceptable. If the wrong order is used, an error message is printed and the program aborts.

Example: POINT, P, 10, T, 2500

31. PRL [PRint Limiter]

Form: PRLimit, CON, 0 | 1 | 2, FIT, 0 | 1, ERR, 0 | 1, PAG, 0 | 1

Description: This instruction controls the amount of output printed by BLAKE. The order of the keywords is immaterial but they must be typed exactly as shown. For example, do not use PAGE for PAG. The numbers have the following significance:

a. CON, 2: Prints the list of constants of the empirical equations for the thermodynamic data of each constituent. This list is printed once after a COMposition instruction is entered provided PRL, CON, 2 has been specified. The list is not printed again for successive COMposition instructions unless and until another PRL, CON, 2 instruction is given; instead the program reverts to PRL, CON, 1.

b. CON, 1: This is the default setting. The list of constants is not printed but the composition of the chamber gas is printed after each GUN instruction; PRL, CON, 2 reverts to this setting.

c. CON, 0: The printing of both the constants and the composition of the chamber gas is suppressed.

d. FIT, 1: Fits the four quantities, chamber pressure and temperature, and covolume and gamma of the chamber gas, to a cubic polynomial in the loading density. The fitting is done provided at least four loading densities are called for in the GUN instruction.

e. FIT, 0: Suppresses the fitting, no matter how many loading densities are called for. This is the default setting.

f. PAG, 0: Inserts a form feed (ASCII 12 = hex 0C) plus additional output at the top of the output for a new run; but thereafter only when a page is filled, or when a new COMposition instruction is entered. The additional output consists of a title (if one was entered), the system date, the BLAKE version designator, and a page number. This is the default setting.

g. PAG, 1: Inserts the additional output for each distinct part of the output from a GUN instruction. These parts are the composition (including the list of thermodynamic constants if called for), the thermodynamic functions for the chamber gas, and the summary. Each output page produced has its own title (if one was entered), the system date, and the version designator.

h. ERR, 0: Suppresses the printing of error messages 28 and 30 (see Sec. X B 28, 30). A summary of the total number of occurrences of each error is printed at the end of the case. This is the default setting.

i. ERR, 1: Prints each occurrence of error messages 28 and 30 as it occurs.

Not all of the parameters on a PRL instruction need be specified at once; users need only include the one(s) they want changed. Once set, each parameter of this instruction remains in effect through a run until it is changed.

Examples: PRL, CON, O

PRL, CON, O, PAG, O

PRL, CON, 2, FIT, 1

32. QEX

Forms: QEXplosion

or

QEXplosion, R, <r>, T, <t> [, <num>, <print>]

or

QEXplosion, T, <t>, R, <r> [, <num>, <print>]

or

QEXplosion, T, , R, <r> [, <num>, <print>]

or

QEXplosion, R, <r>, T, , [<num>, <print>]

or

QEXplosion, R, , T, <t> [, <num>, <print>]

or

QEXplosion, T, , R, , [<num>, <print>]

Description: This instruction computes the heat of explosion of a composition at loading density <r> (in grams/cubic centimeter) at one or more freeze-out temperatures centered around temperature <t> (in Kelvins).

The composition must have been entered previously. The order of the sets T, <t> and R, <r> is unimportant, but the values entered for <r> and <t> must correspond to their key letters. The default values for loading density and freeze-out temperature are 0.2 gram/cc and 1500 K, respectively. These values are the ones used if either or both arguments are omitted. If used, <num> and <print> must be in the order specified, and must be the fifth and sixth arguments, respectively. If <num> is 0 or 1, the calculation is executed at temperature <t>. If <num> is greater than 1 and is odd, then the calculation is executed at <num> different temperatures differing by 100 K and centered on <t>. If <num> is even, then the calculation is executed at <num> + 1 different temperatures differing by 100 K and centered on <t>. If <print> is non-zero, then the program also prints the density of the hot gases at each temperature at which the calculation is executed.

The algorithm used is that of Corner.[8] The program executes a POInt computation at the volume 1/<r> and the chosen temperatures.

The working of the algorithm is critically dependent upon the contents of two DATA statements in the subroutine that contain the names and enthalpies of formation of stable final products at 298 K. This list has been selected for compounds formed by the elements carbon, hydrogen, nitrogen, oxygen, boron, potassium, and sulfur. If additional elements are present, appropriate changes must be made to the DATA statements.

---

8. J. Corner, *Theory of the Interior Ballistics of Guns*, J. Wiley & Sons, New York & London (1950).

Examples: QEX
QEX, R, 0.2, T, 1100, 3
QEX, R, 0.05, T, , 3, 1

33. QUIT

Form: QUIt

Description: This instruction (or its equivalent, STOp--see instruction 39 below) should be the final one in every BLAKE run. It causes the program to execute a normal FORTRAN STOP. It is not absolutely necessary because the program will stop when it runs out of input. If you do not include it or STOp, however, be sure that there is at least one blank line at the end of your input; otherwise the program will repeat the last instruction.

Example: QUI

34. RECALL

Form: RECall, <name1>

Description: This instruction recalls the final conditions associated with the state designated by <name1>. If the point has not been saved (see SAVe, instruction 37 below), an error message is printed and the program aborts.

Example: RECALL, POINT1

35. REJECT

Form: REJect, <name1>, <name2>, <name3>, ...

Description: This instruction eliminates from further consideration the constituents whose legal names are <name1>, <name2>,..., . Illegal or undefined names are ignored without error. A maximum of 99 REJects is permitted; illegal or undefined names are included in the count. This limit is very high and is unlikely to be encountered.

Users familiar with previous versions of BLAKE will find that Version 221.3 requires few if any REJects compared to its predecessors; most compositions will run with none at all.

A REJect list usually remains in effect only until a new COMposition instruction is entered. If you want the same list to be in effect for a series of COMpositions, insert a RETain instruction (see the next instruction).

Example: REJ, C(S), C2H, C2N, C, CH

36. RETAIN

Form: RETain

Description: By default, all ORDer, REJect, and ORC lists are deleted when a new COMposition instruction is entered. The RETain instruction makes the program retain all REJect, ORDer, and ORC instructions from one COMposition instruction to another. The effect of RETain is negated by DEStroy (instruction 10 above).

Example: Ret

37. SAVE

Form: SAVe, <name>

Description: BLAKE and TIGER start new thermodynamic calculations from the results of a previous one, except when initialized by a COMposition instruction. Then the program starts from a preset guess that may be far from the final composition. The convergence of a calculation can often be made more efficient by having the program start from the results of an earlier calculation. This is accomplished in advance by using the SAVe instruction. The conditions (including the final concentrations) just computed are saved in memory, and the name <name> is associated with them. Up to 6 points may be saved in this way, and later recalled (see RECall, instruction 34 above). If you try to save more than 6, an error message is printed, and the point is not saved. A name may be reused; however, the new point overwrites the old one.

Example: SAV, POINT1

38. START

Form: STArt

Description: This instruction is held over from previous versions but is no longer active. In order to form the binary library, the separate program FRMLIB (which is included on the distribution disk) must be used; see Sec. VII. If STArt is entered, the program prints an explanatory note and continues to the next instruction.

39. STOP

Form: STOp

Description: This instruction is identical with QUIt (instruction 33).

Example: sto

40. TIME

Form: TIMe, <duration>

Description: This instruction controls the duration of a calculation. The quantity <duration> sets an upper limit in minutes to the length of time permitted to a run before it is automatically terminated; when this happens the program aborts.

The timing is not exact; for example, when <duration> is set to 0.0001, the program still runs for about 7 seconds. When <duration> is set to 1.2 minutes for a calculation that requires 1.5 minutes, the run terminates in 1.33 minutes.

The default limit is 2.5 minutes which is suitable for a 486 machine working at 120 MHz. Whenever <duration> is entered as 0, the program defaults to 2.5 minutes.

Example: Tim, 3

41. TITLE

Form: TITle, <string>

Description: This instruction centers <string> at the top of each section of subsequent output. If <string> is longer than 72 characters, only the first 72 are used.

Example: TIT, This is an example of a 'title' instruction

42. TRANSPORT

Description: This instruction was intended to compute the viscosity and thermal conductivity of a hot gas mixture but was never implemented. Users who need these properties should instead use the NASA-Lewis program CEA. See Appendix B for references.

43. UNITS

Form: UNIts, ENG | SI

Description: The default output units for the GUN instruction for pressure, impetus, covolume, and flame temperature are megapascals, Joules/gram, cubic centimeters per gram, and Kelvins, respectively. If the keyword ENG is used in this instruction, then *additional* output, with these same quantities expressed in pounds-force per square inch, foot-pounds-force per pound-mass, cubic inches per pound-mass, and degrees Rankine is printed. The metric output cannot be suppressed. The keyword SI restores the default output--metric units only.

Example: Units, eng

VI. RUNNING BLAKE

A. Auxiliary Program. In order to run BLAKE on any MS-DOS computer, the program DOSXMSF.EXE must be stored on that computer in a directory that is included in the computer's PATH statement. This program is included on the distribution disk.

B. Storage. BLAKE requires that all input must be stored in the same directory as the program itself, and in a file named BLAKE.IN. There are two outputs, a complete one stored in BLAKE.OUT, and a much shorter one stored in BLAKE.SUM.

C. Default Units.

1. The units for *input* quantities in BLAKE are shown in Table 7:

Table 7. Units Used in BLAKE

Quantity	Unit
energy	Joule
specific energy or enthalpy	Joule/gram
temperature	Kelvin
density	grams per cubic centimeter
pressure	Megapascal

2. *Internally*, BLAKE uses calories, atmospheres, grams per cubic centimeter, and Kelvins as the units of energy, pressure, density, and temperature, respectively.

3. These units can be changed by altering one or more of the constants PCON, VCON, TMCON, TACON, and HCON in the main program. These constants are used throughout the program as conversion factors for pressure, volume, temperature (two factors), and energy. They are now set to 9.8692, 1.0, 1.0, 0.0, and .23901, respectively. Note, however, that changing these factors does *not* change any of the labels in the program's output. Furthermore, such changes will not affect the outputs from the GUN instruction because megapascals and Joules are 'hard wired' into them.

D. Running BLAKE and RUNBL.BAT.

1. BLAKE requires that its input be stored in a file named BLAKE.IN. Its outputs are placed in two files. The complete output is put into BLAKE.OUT; a brief summary of the output from the GUN instruction only is placed in BLAKE.SUM.

2. While the program may be used in this way directly from the DOS prompt, most users will find it more convenient to use the DOS batch file, RUNBL.BAT, which is included on the distribution disk. This file automates and simplifies using the program.

3. RUNBL.BAT is a DOS batch file that facilitates the use of BLAKE.EXE. It is invoked by typing

RUNBL <file> [S | s]

(The notation used here is explained in Sec. V C.)

a. RUNBL must be stored on the same drive and in the same directory as BLAKE.EXE.

b. The input file must be a file named <file>.INP. The extension .INP must be used. The name <file>, however, is completely optional with the user; it may also contain drive or directory designators if desired.

c. RUNBL copies <file>.INP to BLAKE.INP (thereby destroying the previous contents of that latter file). It then runs BLAKE.

d. When the program has finished successfully, RUNBL copies BLAKE.OUT to <file>.OUT, BLAKE.SUM to <file>.SUM, and BLAKE.PLT to <file>.PLT. Finally, a utility named ENHMORE (which is also on the distribution disk) is used to examine either <file>.OUT, <file>.SUM or <file>.PLT, as previously chosen by the user.

e. The use of 'S' (or 's') or 'P' (or 'p') is optional; if one of them is used, <file>.SUM or <file.PLT> is displayed instead of <file>.OUT.

4. If the user forgets the sequence of parameters required by RUNBL, typing

RUNBL

produces a one-line summary on the screen. If more detail is needed but the user prefers not to look up the documentation, typing

RUNBL ?

displays the essence of this section, a screen at a time.

5. Typing

RUNBL E

produces an abbreviated list of the program's error messages. Only upper-case 'E' may be used.

6. Typing

RUNBL I

produces an abbreviated list of the program's instructions. Only upper-case 'I' may be used.

VII. THE INSTRUCTION SET FOR FRMLIB

A. FRMLIB is the program that forms BLAKE's binary libraries from the alphanumeric ones. The instructions used in the alphanumeric library are identical with those used in previous versions of BLAKE; they are repeated here for completeness.

B. The First Line. An important difference between the present version of FRMLIB and all versions of BLAKE prior to 219.1 is that an extra line is required at the beginning of the alphanumeric library. The contents of this extra line are unimportant--even a blank will do--but it is useful to insert in it the date and other identifying information.

C. Details of FRMLIB's Instructions.

The form of the library instructions is the same as those of BLAKE's. They are given here in alphabetical order. Good bookkeeping practice suggests that the library file be kept with all of the instructions for a given product located consecutively; however, this is not necessary--the program sorts the input when the end of the file is reached.

1. CONSTITUENT

Form: CONstituent, <name>, GAS, <el1>, <n1>, <el2>, <n2>, ...

or

CONstituent, <name>, CONDEN, <el1>, <n1>, <el2>, <n2>, ...

Description: This instruction defines <name> as the official name of a constituent. One of the parameters GAS or CONDEN (for 'condensed') must appear. The quantities <el1>, <el2>,..., are the symbols of the elements that appear in <name>. <n1>, <n2>, ...,are the numbers of atoms of those elements, respectively. Note that a condensed constituent may appear in either the liquid state, the solid state, or both.

Examples:
```
CONSTITUENT, H2O, GAS, H, 2, O, 1
CON, K2CO3$, CONDEN, K, 2, C, 1, O, 3,
CONstituent, NA, GAS, NA, 1
```

2. ELEMENT

Form: ELEment, <sym>, <atwt>

Description: This library instruction defines <sym> as the official name of an element whose atomic weight is <atwt>. No constituent name will be accepted by the program unless all of its constituent atoms appear in ELEment instructions. Note that if the element itself is to be allowed as a constituent, it must also appear in a CONstituent instruction.

Example: ELEment, NA, 22.98997

3. END [OF LIBRARY]

Form: END

Description: This instruction marks the end of the library file. Its use is optional; the end-of-file marker serves the same purpose.

Example: End

4. PRINT [The Library]

Form: PRInt

Description: This instruction, which may appear anywhere in the list of library instructions, creates a listing of the library on output unit LO. The listing is not printed unless this instruction is entered. The library listing is ordered according to the order of appearance of the CONstituent instructions and is formatted for easy reading. A copy should be made every time the library is changed.

Example: Pri

5. STC [STate Condensed]

Form: STC, <name>, SOLID, 1, <b1>, <b2>, <b3>
STC, <name>, SOLID, 2, <b4>, <b5>, <b6>
STC, <name>, SOLID, 3, <b7>, <b8>, <b9>
(and similar forms for LIQUID)

Description: The STC instruction supplies data for the equation of state of a condensed substance, either LIQUID or SOLID. The order of the instructions is immaterial, but all three lines must appear; if not, all of the data are skipped. (This will eventually lead to a run-time error when the program tries to take the reciprocal of <b1>.) Also, the three coefficients must appear in the correct order in any given line.

If the phase of a product does not exist (*i.e.*, there are no thermodynamic data for it), then no STC instructions are required for it.

The coefficients themselves belong to the empirical equation

$$V = A_1 + A_2P + A_3P^2,$$

where V is the molar volume of <name>, and the A_i are given by

$$A_1 = b_1 + b_2T + b_3T^2,$$
$$A_2 = b_4 + b_5T + b_6T^2, \text{ and}$$
$$A_3 = b_7 + b_8T + b_9T^2.$$

Here, P and T are the pressure in atmospheres and the temperature in Kelvins. The b_i are represented by the <b*i*> in the instruction. All 9 coefficients will seldom be known for most materials, but zeros must appear in the instructions for all missing coefficients.

Examples:
```
STC, C(S), SOLID, 1, 4.99259,    3.9628E-5,    1.191359E-9
STC, C(S), SOLID, 2, -6.377527E-6, 1.1924995E-10, -3.7557816E-15
STC, C(S), SOLID, 3, 3.58287E-12, -1.00976E-16,   0

STC, NAF$, LIQUID, 1, 18, 0, 0
STC, NAF$, LIQUID, 2, 0, 0, 0
STC, NAF$, LIQUID, 3, 0, 0, 0
```

6. STG

Form: STG, <name>, <cov>, T|E, <t>, S|D, <s>
or
STG, <name>, <cov>, S|D, <s>, T|E, <t>,

Description: This instruction differs from the STG instruction of TIGER. Here <name> is the legal name of a gaseous constituent as defined by a CONstituent instruction. The quantity <cov> is the BKW covolume of this substance, which is not to be confused with the covolume used in the Noble-Abel equation. The program no longer uses the BKW gaseous equation of state, but a place holder (at least a blank) must be inserted in the instruction.

The quantities <t> and <s> are the two Lennard-Jones parameters, the well depth and the molecular diameter. The key letters T and S may be replaced by either E or D, respectively, and their order may be interchanged. Of course <t> and <s> must be associated with the proper key letter.

If one of the Lennard-Jones parameters is specified, then so must the other; if not, neither one is accepted.

Example: STG, CO2, GAS, 600, D, 3.941, T, 195.2

7. STR [STate Reference]

Form:
```
STR, <name>, GAS, 1, <a1>, <a2>, <a3>
STR, <name>, GAS, 2, <a4>, <a5>, <a6>
STR, <name>, GAS, 3, <a7>, <a8>, <a9>
```

Description: These instructions introduce the thermodynamic data for <name> into the library. The keywords LIQUID or SOLID may appear instead of GAS. If a substance forms only a liquid (or solid), then the STR instructions for solid (or liquid) are omitted for that substance.

The coefficients, <*ai*>, are related to the heat capacity at constant pressure, C, enthalpy, H, and entropy, S, by the empirical equations

$$C_P T/R = a_1 + a_2*\Theta + a_3*\Theta^2 + a_4*\Theta^3 + a_5/\Theta + a_6/\Theta^2 + a_7/\Theta^3;$$

$$H(T)/R*T = a_1 + a_2*\Theta/2 + a_3*\Theta^2/3 + a_4*\Theta^3/4 + (a_5*ln\Theta)/\Theta - a_6/\Theta^2 - a_7/2*\Theta^3 + a_8/(R*T);$$

and

$$S(T)/R = a_1*ln\Theta + a_2*\Theta + a_3*\Theta^2/2 + a_4*\Theta^3/3 - a_5/\Theta - a_6/2*\Theta^2 - a_7/3*\Theta^3 + a_9/R,$$

where Θ = T/1000, and R = 1.98719 calorie/mole-K. It is worth emphasizing that the energy unit for C_P, S, and H is the calorie, not the Joule. This is because *internally*, BLAKE uses calories, not Joules.

Only C_p is actually fitted; the other functions are computed using the values of a_1 to a_7 for C_p plus the integration constants, a_8 and a_9. These latter constants are found by fitting H and S, respectively, at T = 298.15. The heat capacities for gases in SBLAKLYB.LIB are fitted from 300 to 6000 K; in XBLAKLYB.LIB they are fitted from 3000 K to 10000 K. Liquids and solids are fitted over physically-meaningful ranges.

Example:

```
STR, H2O, GAS, 1,  5.5667473D+00,  1.2214169D+00, -2.5753613D-01
STR, H2O, GAS, 2,  1.8817043D-02, -2.4580548D+00,  1.0329816D+00
STR, H2O, GAS, 3, -1.3915671D-01, -6.1781157D+04,  4.9503227D+01
```

VIII. RUNNING FRMLIB

A. FRMLIB is executed by the command

FRMLIB < Lib_file >

where < Lib_file > is the name of one of the alphanumeric libraries. Regardless of the input file, the output from the program is a file named BYNLYB.DAT. A user must copy this file to either SBYNLYB.DAT or to XBYNLYB.DAT, as appropriate. The task is simplified by using the batch file, MAKELIBS.

B. MAKELIBS.BAT is a DOS batch file that automates the production of BLAKE's two binary libraries. Only a user who has made any changes in SBLAKLYB.LYB or in XBLAKLYB.LIB will need this batch file. Producing a new binary library requires running FRMLIB on the revised alphanumeric library, and then copying the resulting binary file to SYBNLYB.DAT or XBYNLYB.DAT, as appropriate. MAKELIBS automates these tasks.

C. Details.

1. MAKELIBS has two forms, either

MAKELIBS

or

MAKELIBS < Sfile | N > < Xfile >

2. The first form assumes that the alphanumeric libraries have their default names; namely, the ones furnished on the distribution disk.

3. The second form permits the user to use arbitrary names. In this case, < Sfile > is the name of the file containing the *standard* library; < Xfile > is the name of the file containing the *extended* library. The order of entry of the names of the two libraries is fixed and may not be changed.

4. The sentinel N may be used to skip processing the alphanumeric library. Only N may be used; n will not work.

5. The names of the binary libraries are fixed and cannot be changed by users without making changes in the source codes of FRMLIB and BLAKE, and then recompiling.

6. If an erroneous name is specified for an alphanumeric library, FRMLIB aborts with a run-time error message. Its corresponding binary library is not changed.

7. When MAKELIBS successfully forms a binary library, it prints a note to that effect on the screen.

8. It is possible for one of the two libraries to be formed successfully while the other one is not.

IX. OUTPUT FOR THE SAMPLE CASES

Appendix D presents a series of typical BLAKE inputs. These sample cases illustrate most of the program's instructions; one of them is an example of how to work with a difficult composition. For the most part the inputs are self-explanatory. In a few cases comments are inserted starting in either column 4 or 5 of the input; the program inserts the former, but not the latter, into the output.

The output from these test cases is given in full in Appendix E. The printing of the product concentrations has been suppressed in most cases to save space. The following discussion gives details about the interpretation of the results. The run times printed at the end of each case were obtained using an IBM-compatible 120 MHz-486 computer. Times recorded with a 200 MHz Pentium computer were about 25% as long.

CASE 1. The FORmula, COMposition, and GUN Instructions

When the program starts, it immediately prints an identifying banner. Subsequently each line of input that has at least one non-blank character in cols. 1 - 4 is echoed.

In this case, a FORmula instruction has been entered for a substance whose name (AN) is already in the prestored formulas; a warning message is printed and the new formula replaces the old. This replacement is emphasized in this case because the enthalpy of formation of ammonium nitrate was entered in calories/mole, and the order of the elements is different from that in the prestored formula.

As soon as a valid COMposition instruction has been executed, the program prints an identifying header that includes the contents of the first line of the alphanumeric library (see Sec. VII B) and the date that the binary library was formed.

Then the details of the composition are printed. For each ingredient, its name, percent by weight, percent by mole, enthalpy of formation (in Joules/mole) and formula are printed. Next the elements and their atom percentages are printed, followed by the formula weight of the composition.

Note that the formula weight printed, 889.356, corresponds to the molecular formula $N_{22.222}O_{33.333}H_{44.444}$ and so is quite different from 80.043, the formula weight corresponding to $N_2H_4O_3$. The molar heat of formation printed in the next line is based on the formula weight 889.356. This example is trivial because it is easy to spot the multiplier 11.111 in the listing of the atomic percentages; it is not so easy for a typical propellant mix as later examples will show.

Next the GUN instruction is executed. Inasmuch as no print-limiting instruction was entered, the default condition is the printing of the equilibrium concentrations of the product species in moles per kilogram of mix. In this case the GUN instruction requested computations at 8 different loading densities; the corresponding outputs are labelled '1)', '2)', ... If more than 4 loading densities are specified, the next set of four appears immediately following the first four. Regardless of how many loading densities are specified, no more than 32 are printed for any one GUN instruction. All of the final concentrations of the gaseous products are printed first, followed by those of the condensed species.

The SUMMARY of the GUN output is the final output. It lists 10 quantities as follows:

RHO/L (= Loading Density). The ratio of the total mass of the propellant mix (or charge) to the geometric volume of the chamber in grams per cubic centimeter. Many ballistic performance codes use thermochemical data computed for a loading density of 0.2 g/cm^3 as their reference values. BLAKE results for loading densities greater than about 0.4 g/cm^3 are of dubious validity and should be used with great caution if at all.

Temp (= Temperature). BLAKE calculations always assume that there is no heat loss. This temperature (in Kelvins) is the theoretical maximum equilibrium value that the system can reach under such conditions. It is sometimes referred to as the adiabatic flame temperature, T_V.

Press (= Pressure). The equilibrium chamber pressure in megapascals.

Imptus(= Impetus). Consider a mass of propellant, *W*, in a chamber of volume *V*. At theoretical equilibrium conditions in this chamber, there will be gaseous products of average molecular weight *M*; there may also be condensed products of mass *w*. The impetus of the propellant is defined as

$$\text{Impetus} = [(W-w)/M] \cdot R \cdot T_V,$$

where

T_V = adiabatic flame temperature,

and

R = universal gas constant (= 8.314 J/mol-K)

Most gun propellants do not form condensed products at chamber conditions, so $w = 0$, and impetus is then simply $(W/M) \cdot R \cdot T_V$.

Mol Wt (= Molecular Weight (gas)). The quantity *M* just defined. Note that it refers solely for the gas phase, not to all of the products.

Co-Vol (= Co-Volume). The quantity *b* in the Noble-Abel gaseous equation of state,

$$p(V - Wb) = [(W-w)/M] \cdot R \cdot T.$$

Its units are cubic centimeters per gram. (See Hirschfelder *et al.* (Ref. 7) or Maitland *et al.*[9] for a discussion of nonideal gaseous equations of state.)

Frozen gamma. This is the ratio of the two frozen heat capacities, C_p/C_V. It is frequently used in ballistic performance codes.

Balrgy (= Ballergy). This is another word for *ballistic energy*, formerly called the *chemical energy*.It is defined by

$$\text{Ballergy} = \frac{\text{Impetus}}{\gamma - 1}$$

where $\gamma = C_p(frz)/C_V(frz)$, the frozen gamma defined above.

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9. Maitland, G.C., M. Rigby, E.B. Smith, and W.A. Wakeham, *Intermolecular Forces: Their origin and determination*, Oxford University Press (1981), Chap. 3.

U (= Internal Energy). This is 'energy' printed by the COMposition instruction.

PHI. The compressibility factor, defined as the ratio of the nonideal gas pressure to the ideal gas pressure for the same conditions. The physical significance of BLAKE results decreases with increasing values of PHI, but this statement cannot be quantified.

The SUMMARY also appears on the screen and is placed in the file BLAKE.SUM.

CASE 2. The MORe, BPR, and UNIts instructions

This case is a variant of Case 1. In addition to the basic input--title, composition, and gun instructions--there are 3 more that produce additional output. The first part of the SUMMARY was discussed previously. The MORe instruction prints six more quantities. For the user's convenience the loading density, temperature, and pressure are repeated. They are followed by six additional quantities:

Cp(Frz), which is the frozen heat capacity at constant pressure.

B(T) and *C(T)*, which are the second and third virial coefficients, respectively. They are used in the truncated virial equation,

$$PV = nRT\cdot[1 + nB(T)/V + (n/V)^2C(T)].$$

(See Refs. 7 and 10 for further discussion.) The units of B(T) and C(T) are cubic centimeters/mole and (cubic centimeters/mole)^2, respectively.

S, which is the entropy of the hot gas mixture in the chamber; its units are Joule/mole-K.

Gas Vol, which is the specific volume of the chamber gas mixture in cm^3/g. If there are no condensed phases in the chamber, then the specific gas volume is just the reciprocal of the loading density. But if there is one or more condensed phases, then the specific volume of the gas phase will be a larger number than the reciprocal of the loading density. And last,

AdExp, which is the adiabatic exponent, defined by

$$\text{AdExp} = -(\partial \ln P/\partial \ln \rho)_S.$$

The UNIts instruction causes the printing of the same quantities in conventional (English) units. Even those who prefer these units for pressure, impetus, and co-volume nevertheless refer to loading density in g/cm^3, as is done here.

The instruction BPR creates a separate file, VIRIALS. For ease of reference, however, its contents are appended to the end of the output for CASE 2 in Appendix E. Each GUN calculation adds 6 lines to VIRIALS. The first line is the title of the particular case. The second line gives the final temperature and the second and third virial coefficients

for the mixture. The units of these quantities are not printed, but are cubic centimeters per mole and (cubic centimeters per mole)^2, respectively. The remaining lines give the second virial coefficient for 16 gaseous products formed by any propellant containing C, H, N, and O. If there is only one GUN instruction, but it calls for computations at more than one loading density, then the output in VIRIALS is for the final density only.

CASE 3a. An unsuccessful black powder calculation

In this example, the instruction PRL, CON, 2 makes the program print the products' thermodynamic data that will be used in the calculation. Data for the gaseous products come first, followed by those for the condensed products. For gases these data are as follows (from left to right): The name of the product, its BKW co-volume, its Lennard-Jones reduced temperature and diameter, and then the 9 constants for the fitting of the heat capacity, entropy, and enthalpy (these are the a_i discussed in Sec. VII C 7). Note that the BKW co-volume is not used in this version of BLAKE.

Next the value of the floor, which is discussed in Appendix A, is printed. Then the thermodynamic and thermophysical data for possible condensed products (if any) are printed. Potentially 36 constants may be required to represent the data for the liquid and solid phases of one species, $9 \times 2 = 18$ for the thermodynamic data for 2 phases, and an equal number to describe their P-V-T behavior. Only carbon has all 9 constants known for its solid equation of state.

The names of the various species may not have more than 6 characters, which are not always enough to identify them. The heading FRMS IN LIB PRT means that the full formulas for the chosen condensed species may be found in the printout produced by FRMLIB (see Sec. VII). In the condensed-phase display the constants for the thermodynamic data are given first for the liquid phase and then for the solid phase. These are followed by the constants for the liquid/solid equation of state; these are the b_i described in Sec. VII C 5.

The computation of the equilibrium thermodynamic properties of the hot gases produced by black powder is a difficult problem for BLAKE because the final mixture contains two or three species in condensed phases. In this particular example the computation fails to converge. An examination of the possible products for this case shows that the program selected 5 condensed-phase species (C(S), KOH$, $K_2CO_3$$, $K_2S$$, and $K_2SO_4$$) which it can rarely, if ever, handle correctly. Rather than resort to cut-and-try methods, the NASA CEA program (see Appendix B) was used for guidance. In the general case, the output from CEA can guide the user not only for REJect instructions, but also ORder and ORC instructions. In the present case, the additional instruction, REJ, C(s), KOH$ was sufficient, as shown in the next case.

CASE 3b. A successful black powder calculation

Case 3b deals with the same compostion as Case 3a, but with the guidance from CEA, the species KOH$ and C(S) have been rejected. The program is now able to complete the computation, albeit slowly, for all of the specified loading densities.

Examination of the results for this case shows a peculiarity for the loading densities 0.00010 and 0.00020 g/cm^3. The obvious indication that something is wrong with this output is the '*******' printed in place of the co-volume, showing that the value exceeds the allotted space. A further indication is the fact that the printed value for the internal energy, U, is not the input energy which *must* be -4139.6 J/g as already printed previously. The anomalous output in this case has never been observed with any other composition. Paul Baer* has studied this problem intensively and has shown that it arises from the algorithm used in finding the equilibrium composition.

CASE 3c. A better black powder calculation

In the course of his investigation into the the difficulties with black powder calculations, Baer found that using a negative increment in the GUN instruction removed the anomaly most of the time, as shown in this example.

CASE 4. The BOMb (closed-bomb) instruction

This instruction is a variant on the GUN instruction. The form of the output is the same as that from the GUN instruction.

CASE 5. A GUN calculation, then an isentropic expansion

The entropy, which will be held constant, is that of the hot gas in a closed bomb or gun chamber. It is computed using the GUN instruction; then an ISOline instruction is executed. It is not necessary to copy the entropy into the ISOline instruction: the program does it by means of the 'double comma' feature.

The quantities printed in the first part of the output are the same as those printed for the GUN instruction. The output from the ISOline instruction consists of 13 quantities displayed in 2 rows. The first row consists of the pressure, specific volume, temperature, specific enthalpy, specific energy, specific entropy, and density of the equilibrium mixture. The second row consists of the specific heat at constant volume, and 5 additional quantities:

Alpha and *Beta* are the derivatives $(1/P)(\partial u/\partial V)$ and $(1/V)(\partial u/\partial P)$, respectively. They arise in the computation of the thermodynamic properties of reacting gases but are not used in the ballistic computations. See pp. I-60, 61 of ref. 1 for further details.

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* Paul Baer, USA BRL, retired. In several private communications to E. Freedman, November 1997-January 1998, he showed that the problem arises specifically in the Newton-Raphson technique the program uses to solve a set of strongly non-linear equations. The problem becomes increasingly more severe at lower loading densities, as is shown by oscillations in a plot of co-volume against loading density. Baer was ultimately able to get physically reasonable results and a smooth co-volume plot by using a decrement of -0.0625E-4 in the loading density.

AdExp is the adiabatic exponent, defined by

$$\text{AdExp} = -(\partial \ln P / \partial \ln \rho)_S .$$

Sigma is one of the Riemann integrals,

$$\text{SIGMA} = -\int_{a_1}^{a_2} c_1 da$$

where c_1 is the local sound speed, and a(i) is $\log_e$ (v(i)).

Omega is the other Riemann integral,

$$\text{OMEGA} = -\int_{a_1}^{a_2} c_1^2 da$$

CASE 6. A POInt calculation--constant pressure flame

This example is the computation of the isobaric flame temperature of a propellant. In order to compute the initial enthalpy of the mixture, a COMposition instruction is executed first. In this case the user must copy the computed enthalpy manually to the next instruction; no provision exists for the automatic transfer as there was with the ISOline instruction. The thermodynamic properties computed by the POInt instruction have already been defined.

CASE 7. Electrothermal GUN calculation with 2 libraries.

The GUN instruction, as noted in Sec. V D 19, permits the user to specify an arbitrary amount of electrical energy to be added to the system. In this example, the propellant being studied is JA2, which is one of the prestored propellant compositions. When the program determines that additional energy has been specified, it prints the modified heat of formation, which is the sum of the initial heat of formation plus the added energy. From then on the output is similar to that for Case 1.

In this example, the LIB instruction is used to call for the extended (high temperature) library, and then the computation is repeated.

CASE 8. A heat of explosion calculation.

The instruction for this case specifies a calculation of the heat of explosion at the default density, 0.2 g/cm^3, and for 5 assumed freeze-out temperatures (T_f) centered around 1500 K. (Whenever an even number of T_f's is given, the program always adds 1.)

The appearance of 'P' in the instruction specifies that additional output is wanted. The first output (after the composition of the gas mixture at the selected T_f) is the loading density, and then the gas density with solids excluded. Note that at four of the five temperatures selected, solid carbon is formed; hence the gas density is greater than the loading density. The computed pressure at the assumed T_f is printed next. Then the principal output, the heat of explosion, is printed. Finally, a parenthetical note is appended that specifies what percentage of the equilibrium products have been accounted for in the computation. This number will always be greater than 99% for C, H, O, and N mixtures; it may be less for mixtures containing other elements.

Case 9. Forming a plot file

Several different computations are included in this case. Their plot outputs are all combined in the same file, BLAKE.PLT, which is printed in Appendix E. The principal output for this case is omitted.

The contents of this file are described in Sec. V D 29.

X. ERRORS AND WARNINGS

A. Introduction.

1. Errors are *always* fatal: A descriptive message is printed and the program halts whenever one is encountered. (This is a change from previous versions.) Warnings indicate a possible problem. Often (*e.g.*, nos. 28 and 30 below) they indicate that the computation is having difficulty in finding the equilibrium point; if equilibrium is reached, however, then they have no significance so they are usually not printed (see the discussion of the PRL instruction in Sec. V). Other times (*e.g.*, nos. 47a and 47b) they indicate that caution should be exercised in interpreting the results.

2. BLAKE and FRMLIB together contain 48 error messages or warnings mostly taken over from TIGER. Most of them (*e.g*, nos. 1-5, 10 below) are useful in detecting problems. A few, however, (*e.g.*, nos. 6, 7 below) are not helpful to the typical user who only wants answers and is not interested in the tedious details of why convergence was not reached. Errors and warnings will be considered together in the following descriptions.

B. Details about the Error and Warning Messages.

The exact wording of each error or warning message is given below, followed by an explanation of its significance if one is needed. In most instances, the steps to be taken to avoid the problem will be obvious; in a few cases additional discussion is given. Error messages arising from improperly-typed instructions are generally accompanied by a repeat of the offending instruction.

1. *ERROR #1: Unknown instruction.* Table 6 in Sec. V gives a list of the 43 accepted instructions in BLAKE. Any other instruction gives rise to this message.

2. *WARNING #2: Too many constituents REJected.* The program permits a maximum of 99 products to be rejected. This limit will seldom if ever be exceeded.

3. *WARNING #3: Too many constituents ORDered.* The program permits a maximum of 25 products to be ordered. In theory the number of products ordered need not exceed the number of different elements in a system. Even if a system has 10 different elements (highly unlikely) and the user orders 2 possible products for each of them, only 20 products are involved.

4. *WARNING #4: Too many constituents CHOsen.* The limit here is also 25 and is also unlikely to be exceeded because rarely if ever does a system form as many as 15 significant products.

5. *WARNING #5: GEO instruction is faulty.* See Sec. V D 17 for the list of acceptable KEYWORDS. The program will default to using the virial equation.

6. *WARNING #6: Finding RHO0: Excessive iterations.* This warning tells the user that the program was having trouble converging. This particular message is rare: Convergence difficulties more often result in errors 28 or 30.

7. *WARNING #7: Finding T0: Excessive iterations.* See the discussion for Warning 6.

8. *ERROR #8: Components linearly dependent in SELECT.* This message is extremely rare. No example of its occurrence is available. It would probably arise if the product library contained, for example, both KO and K_2O_2.

9. *ERROR #9: No acceptable components in SELECT.* This message is not as rare as #8, but it never arises when working solely with systems containing only C, H, N, and O; and never with systems that do not form condensed species. When it does occur, however, the user's best recourse is to use one of the NASA-Lewis thermodynamics programs (see Appendix B) for guidance in selecting ORder and ORC instructions.

10. *ERROR #10: Bad FORmula instruction.* This message is caused most often by typographical errors. A FORmula instruction involving an element not in the program's library will also result in this message.

11. *ERROR #11: EXPlosion instruction not acceptable.* See the format of the EXPlosion instruction in Sec. V D 12 and 13.

12. *ERROR #12: Input to POInnt not acceptable.* See the discussion of the POInt instruction's format in Sec.V D 30.

13. *ERROR #13: This point not saved.* This is self-evident.

14. *ERROR #14: Too many points saved..* This is self-evident. A maximum of 6 points may be saved.

15. *ERROR #15: No COMposition instruction in QEXp.* This is self-evident.

16. *ERROR #16: [In FRMLIB.] Library instruction not acceptable.* This is self-evident. (Note that Message #1 arises only in BLAKE, while the present message arises only with FRMLIB.)

17. *ERROR #17: This COMposition instruction not acceptable.* This is self-evident. Note that when Error #18 occurs, it is often soon followed by the present message. Once this error has occurred, the program will not process any further computational instructions until a valid COMposition instruction has been entered.

18. *ERROR #18: FORmula name not in table.* This message arises if a formula cannot be found when a COMposition instruction is being executed.

19. *ERROR #19: No COMposition instruction in GUNCAL.* The GUN instruction checks whether a valid COMposition instruction has been entered.

20. *ERROR #20: Not all ORDered constituents in library.* A possible product may not be rejected unless it actually occurs in the library. This error may arise when the product is in fact in the library, but the user has not entered the correct name; for example, typing HBO instead of BHO.

21. *ERROR #21: Freeze matrix singular.* This error is fatal.

22. *ERROR #22: Freeze force iteration exceeded.* This error usually signals an end to the particular calculation.

23. *WARNING #23 Freeze iteration exceeded.* This error is sometimes encountered during a frozen ISOline calculation. Often it merely indicates a minor holdup in the calculation.

24. *ERROR #24: Thermo iteration exceeded in either ECOMPO or THERMO.* This message is fatal. When it occurs, users must reconsider their approach to the computation that gave rise to it. Recourse to the NASA-Lewis thermodynamics program is suggested. See Appendix B.

25. *ERROR #25: Time limit exceeded in ECOMPO.* See the discussion of TIMe in Sec. V D 40.

26. *WARNING #26:* Withdrawn.

27. *ERROR #27: In ECOMPO: Singular matrix when solving for ETAs.* This message is rare. The only occasion in which it arises is, for example, in a system such as a mixture of NO_2 and N_2O_4 in which the formation of the equilibrium products N_2 and O_2 has been prohibited.

28. *WARNING #28: Solving for ETAs excessive iterations.* This and Warning #30 are the two most commonly encountered errors during a calculation; they indicate problems in attaining convergence. In most cases convergence is eventually reached so little is gained by having them printed repeatedly; therefore, the program's default setting is that neither message is printed. If, however, convergence is not reached, a

summary of the total number of times each error occurred is printed. See the discussion of PRL in Sec. V D 31.

29. *ERROR #29: In ECOMPO: Singular matrix when solving for N(I)s.* This error message is rare.

30. *WARNING #30: Solving for N(I)s excessive iterations* See the discussion of Error # 28 above.

31. *ERROR #31: Too many gaseous constituents selected: (...) chosen, but only 56 are permitted.* The present version of BLAKE has a smaller library and permits a larger number of possible products than did any of its predecessors. Consequently this error message is unlikely to be encountered; if it is, REJect instructions must be entered.

32. *ERROR #32: Too many condensed constituents.* The theoretical maximum number of permitted condensed constituents is 10; unfortunately, the program rarely converges if as many as 4 condensed constituents are present. The only solution is to enter REJect instructions.

33. *WARNING #33: [In FRMLIB] Too many ELEment instructions.* The limit is now 40. There are only 21 elements in the current BLAKE library; users may add up to 19 more.

34. *WARNING #34: [In FRMLIB] Too many CONstituent instructions.* This means that the user has entered more CONstituent instructions than the number for which the program is dimensioned. The present limit is 180, of which 111 are supplied in the current BLAKE library.

35. *WARNING #35: [In FRMLIB] Too many STG instructions.* This means that the user has entered more STG instructions than the number for which the program is dimensioned. The present limit is 100; only 23 are currently entered.

36. *WARNING #36: [In FRMLIB] Too many STR instructions.* This means that the user has entered too many STR instructions. The present limit is 1218; only 333 are presently entered.

37. *WARNING #37: [In FRMLIB] Too many STC instructions.* This means that the user has entered too many STC instructions. The present limit is 180; only 72 are presently entered.

38. *ERROR #38: UNIts instruction is faulty.* This is self-explanatory; see also the discussion in Sec. V D 43.

39. *ERROR #39: GUN instruction has misfired.* This is self-explanatory.

40. *ERROR #40: No valid COMposition instruction has been entered.* This error message will occur if a computational instruction is entered without a previous COMposition instruction (Note that GUN has its own error message in this case.)

41. *ERROR #41: Formula elements not in library.* This error occurs when the user attempts to use BLAKE's extended library on a composition that has elements other than C, H, N, and O in it. A subsequent computational instruction may execute, but the results will not be valid. Note that this is an error in BLAKE, not in FRMLIB.

42. *ERROR #42: [In FRMLIB] Two or more elements have the same name.* This is self-evident.

43. *WARNING #43: [In FRMLIB] Two or more constituents have the same name.* This also is self-evident.

44. *WARNING #44: Element ... is not in array ELMTS. The program continues, but the computed Formula Weight and the Molar Heat of Formation will be in error.* This error can arise only if the program's library has been modified by the addition of one or more elements without also making the appropriate modification to the array ELMTS in the BLOCK DATA subprogram.

45. *ERROR #45: Binary library file not in current directory.* The program checks that the binary library file exists before opening it. If the file is missing or, more likely, in the wrong directory, the program aborts with this message.

46. *ERROR #46: Input to ISOline is incorrect.* Self-explanatory.

47. *WARNING #47a: Your requested freeze-out temperature ... is greater than 3500 K. Use caution when interpreting the results.* Specifying a freeze-out temperature greater than the adiabatic flame temperature is physically meaningless.

WARNING #47b: Your requested freeze-out temperature ... is less than 298 K. Use caution when interpreting the results. The lower temperature limit of the fitting of the thermodynamic data in the program library is 298.15 K. Extrapolation below this limit is risky. Also, on physical grounds, it is unlikely that computing freeze-out properties at temperatures below about 1000 K is meaningful.

48. *ERROR #48: Zero increment in ISOLINE instruction is not permitted.* Self-evident.

XI. REFERENCES

1. Blake is based on the original version of TIGER that was developed by Stanford Research International under Contract No. DA-04-200-AMC-3226(X) with the (former) US Army Ballistic Research Laboratories. Dr. Stanley M. Taylor was the Contracting Officer's Technical Representive. This work was documented in an SRI report by Wibenson, W.E., Jr., Zwisler, W.H., Seely, L.B. and Brinkley, S.R., Jr., "Tiger Computer Program Documentation", 1968.

2. A revised and improved version of TIGER is documented in Cowperthwaite, M., and Zwisler, W .H., "Tiger Computer Program Documentation," SRI Publication No. Z106, 1973.

3. Freedman, Eli, "Blake--A Thermodynamics Code Based on Tiger--Users' Guide and Manual," ARBRL-TR-02411, 1981 [AD A121 259]. An errata list for that report is given in Appendix F of the present report.

4. The development of the extended library is discussed in detail in Oberle, W.F. and Freedman, Eli, "Preparation and Extension of the Thermodynamics Program BLAKE and Its Library to 10,000 K for Use with Electrothermal-Chemical (ETC) Systems," ARL-TR-488 (July 1994).

5. Kotlar, A.J., "The Effect of Variable Composition Equilibrium Thermochemistry in Constant Breech Pressure (CBP) Gun Simulations," *Ballistics '95: 15th International Symposium on Ballistics (Proceedings)*, IB16, Vol. 3, pp 119-126; 1995.

6. Kotlar, A.J., US Army Research Laboratory. Private communication to Eli Freedman, June 1995. This technique is used implicitly in his paper, Kotlar, A.J. "The Thermodynamics of Interior Ballistics and Propellant Performance," *Proceedings, 29th JANNAF Combustion Conference*, CPIA Publication 593 (October 1992). In reading this paper, the designations static and dynamic are used for freeze and melt. This must be kept in mind in order to read the tables correctly.

7. Hirschfelder, J.O., C.F. Curtiss, and R.B. Bird, *Molecular Theory of Fluids*, John Wiley & Sons, New York (1954), Chap. 3.

8. Paul Baer, USA BRL, retired. Private communication to E. Freedman, 15 November 1997.

9. J. Corner, *Theory of the Interior Ballistics of Guns*, J. Wiley & Sons, New York & London (1950).

10. Maitland, G.C., M. Rigby, E.B. Smith, and W.A. Wakeham, *Intermolecular Forces: Their origin and determination*, Oxford University Press (1981), Chap. 3.

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Appendix A.

COMMENTS ON THE COMPUTATION OF EQUILIBRIUM BY TIGER

To shorten the discussion required for some of the instructions, some comments on the philosophy of TIGER's calculation of the equilibrium state will be useful. The discussion will be entirely qualitative; the complete technical details are in the TIGER manuals. [1]

TIGER proceeds by considering at first only those gaseous constituents that are chemically-possible products of the specified mixture. Condensed phases are usually, but not always, considered later if necessary. At each step the program tries to work with a set of N linearly-independent constituents that are present in the largest amounts, where N is the number of different elements present in the mixture. These N constituents are called the *components*. Most of the computing time is spent looking for the correct set of components, which may change with conditions, (*e.g.*, pressure or temperature) even while computing a single composition.

In theory but not in practice the program could permute all of the constituents present until it finds the components. The first attempt at finding the components consists of selecting a linearly-independent set of N constituents as they are retrieved from the library file. This order was determined by the order of the CONstituent instructions in the alphanumeric library at the time the library file was created. For the elements C, H, O, and N, the components usually turn out to be CO2, H2O, N2, and CO, which are therefore the first four constituents in the BLAKE alphanumeric library. This order may be changed by the instructions ORDer and ORC.

If the first selection of components proves to be wrong, the program does some permuting among the constituents. Since one knows chemically that some of the constituents will rarely if ever be present in large enough concentrations to be components, the program makes provision for skipping them. Constituents that are never to be considered as components have an asterisk (*) typed as the last field in their CONstituent instructions. When the program prints the list of constituents selected, those that cannot be components are all printed after those that may be. The dividing line between these two groups is called the *floor*. The user has the capability of raising or lowering the floor by using the instruction FLOor.

BLAKE is presently limited to considering a maximum of 56 gaseous constituents for any one composition. Error message 31 is printed if more than this maximum is selected and the case is rejected. This number is large enough so that REJect instructions will seldom be required.

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1. See Wibenson, W.E., Jr., Zwisler, W.H., Seely, L.B. and Brinkley, S.R., Jr., "Tiger Computer Program Documentation", 1968.

The selection of species to be included in the library was guided by the results of computations using the NASA-Lewis program, CEC86. In general only species that will almost always be present with mole fractions greater than about 1×10^{-4} were selected. As a result there will not be many occasions when the REJect instruction will be needed for gaseous species. This is not the case, however, when many condensed species are possible products. See Case 3b in Sec. IX for an example.

Convergence is materially aided if you have advance knowledge of the major constituents in the equilibrium composition. Such knowledge is often obtained by running the same composition with another code. The NASA-Lewis equilibrium code CEA (see Appendix B) is recommended for this purpose.

Appendix B.

REFERENCES FOR AND COMMENTS ON THE NASA-LEWIS THERMODYNAMICS PROGRAMS

NASA's Lewis Laboratory in Cleveland, Ohio has produced a series of outstanding equilibrium thermodynamics programs over the years. The original one was "CEC" (Chemical Equilibrium Code), which was described in Gordon, Sanford and McBride, Bonnie J., "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouguet Detonations," NASA SP-273 (1971). This report is out of print. NTIS sells an abbreviated version, marked "interim revision," as N78-17724. This code did not compute transport properties.

That feature was added in 1973 to a program named "TRAN72." See Svehla, Roger A. and McBride, Bonnie J., "FORTRAN IV Computer Program for Calculation of Thermodynamic and Transport Properties of Complex Systems," NASA TN D-7056 (1973). (Available from NTIS as N73-15954.)

Later revisions of the program were named "CET86" (Chemical Equilibrium and Transport), "CET89," and "CET93". See McBride, B.J., M.A. Reno, and S. Gordon, "CET93 and CETPC: An Interim Updated Version of the NASA Lewis Computer Program for Calculating Complex Chemical Equilibria with Applications," NASA Technical Memorandum 4557 (1994).

The latest version, CEA (Chemical and Equilibrium Analysis), is described in Gordon, S. and B.J. McBride, "Computer Program for Calculation of Complex Chemical Equilibrium Compositions and Applications. I. Analysis," NASA Reference Publication 1311 (1994); and McBride, B.J. and Gordon, S., "Computer Program for Calculation of Complex Chemical Equilibrium Compositions and Applications. II. Users Manual and Program Description," NASA Reference Publication 1311 (June 1996).

One of the principal features of all of these programs is that from the beginning they have had the capability of handling with ease large numbers of reaction products. From 1973 on, these limits have been 600 gaseous and 400 condensed reaction products.

Whenever BLAKE has trouble executing computations on any composition, the best guidance a user can get is to run the same composition with one of the NASA programs (any one from 1973 onwards). By studying the output, the user can quickly develop a list of REJects, ORDers, and (especially) ORC instructions.

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Appendix C.

BLAKE'S PRESTORED FORMULAS

BLAKE contains prestored formula data for many frequently-used propellant ingredients, as well as a few "single-formula" representations of some frequently-used compositions. The ingredients are referred to by their generally-accepted names or abbreviations.

Table C1 lists these abbreviations alphabetically and gives their chemical names. Table C2, which is arranged in order of the abbreviations, gives the chemical formulas, formula weights, and heats of formation of these ingredients or compositions. The data for all compounds in this table except those for the nitrocelluloses come from Pedley and Rylance [1]. The data for the nitrocelluloses are based on an unpublished reworking of Jessup and Prosen's [2] data. To save space, the entries for NC1123 - NC1400 have been omitted here. Besides being in the program, they are also contained in the distribution disk in a file named FORM_PRT.TAB.

The thermodynamic input for any constant-volume calculation such as a GUN calculation is, strictly speaking, the *energy*. Tables of thermodynamic data (*e.g.*, the *JANAF Tables*[3] or Pedley and Rylance), however, tabulate only enthalpies. The relation between energy and enthalpy, and their relation to tabulated enthalpies of formation is discussed by Kotlar[4], who shows that for solids and liquids, there is virtually no numerical difference between these two quantities. This is not true for gases, where the difference between energy and enthalpy is -2478.9 Joule/mole. Hence, for constant-volume calculations on gaseous reactants, the proper energy input is the enthalpy of formation + 2478.9 J/g. The only gases whose formulas are prestored in BLAKE are the four elements helium, argon, hydrogen, and oxygen, for which different abbreviations are used to distinguish the two cases. For all constant pressure calculations, the correct inputs are HEP, ARP, H2P, and O2P. For constant volume calculations, the correct inputs are HEV, ARV, H2V, and O2V.

Throughout this report and in BLAKE output, the term "heat of formation" is used to specify either energy or enthalpy, whichever is appropriate to the case in hand.

---

1. Pedley, J.B. and Rylance, J., *Sussex-N.P.L. Computer Analyzed Thermochemical Data: Organic and Organometallic Compounds*, University of Sussex, Sussex, 1977.

2.Jessup, R. S. and Prosen, E. J., *J. Res. National Bureau Stds.* 44, 387-393 (1950).

3.JANAF Thermochemical Tables, 3rd edn., ACS/AIP (1986); also, Supplement No. 1 to the *Journal of Physical and Chemical Reference Data*, vol. 14, 1986.

4. Kotlar, A.J., *The Proper Interpretation of the Internal Energy of Formation Used in Thermodynamic Equilibrium Calculations*, BRL Memorandum Report BRL-MR-3985 (1992).

Table C1. Abbreviations and Chemical Names of the Prestored Ingredients in BLAKE

Abbreviation	Chemical Name
ACETON	Acetone (ethyl ketone)
AKAR1	Akardite 1 (diphenylurea)
AKAR2	Akardite 2
AKAR3	Akardite 3
AKARD	Akardite
ALC	Ethanol (ethyl alcohol)
AMYLPH	Amyl phthalate
AN	Ammonium nitrate
ARP	Argon (constant pressure)
ARV	Argon (constant volume)
BANITR	Barium nitrate
BAO	Barium oxide
C	Carbon (graphite)
CEDAC	Cellulose diacetate
CETAC	Cellulose triacetate
CRY	Cryolite (sodium cryolite)
DBP	Butyl phthalate
DECA	Decalin
DEGDN	Diethyleneglycol dinitrate
DNT	Dinitrotoluene
DPA	Diphenylamine
EC	Ethyl centralite
EGLY	Ethylene glycol
EOAN	Ethanolamine nitrate
ETHER	Ether (Ethyl ether)
ETOH	Ethanol
H2O	Water (liquid)
H2P	Hydrogen (constant pressure)
H2V	Hydrogen (constant volume)
HAN	Hydroxylammonium nitrate
HEP	Helium (constant pressure)
HEV	Helium (constant volume)
HMX	Cyclotetramethylene tetranitramine (octogen)

Table C1. Abbreviations and Chemical Names of the Prestored Ingredients in BLAKE (continued)

Abbreviation	Chemical Name
HNO3	Nitric acid
IPAN	Isopropylammonium nitrate
JA2	Propellant JA2
KN	Potassium nitrate
KS	Potassium sulfate
MC	Methyl centralite
METRIO	Metriol
MGO	Magnesium oxide
N2P	Nitrogen (constant pressure)
N2V	Nitrogen (constant volume)
NCvwxy	Nitrocellulose with vw.xypercent Nitrogen
NDPA	2-nitrodiphenylamine
NG	Nitroglycerin (glyceryl trinitrate)
NNDP	2,2-dinitrodiphenylamine
NQ	Nitroguanidine
O2P	Oxygen (constant pressure)
O2V	Oxygen (constant volume)
PB2CO4	Basic lead oxide
PBO	Lead oxide (see also basic lead oxide)
PETN	Pentaerythritol pentanitrate
RDX	Cyclo-1,3,5-trimethylene-2,4,6-trinitramine
TATB	Triaminotrinitrobenzene
TEAN	Triethanolammonium nitrate
TEGDN	Triethyleneglycol dinitrate
TMAN	Trimethylammonium nitrate
TRIAC	Triacetin
WATER	Water (liquid)
XM46	Liquid propellant XM46

Table C2. Formulas, Heats of Formation, and Formula Weights of the Prestored Ingredients in BLAKE

	BLAKE Name	Heat of Formation (J/mol)	Formula Weight	Formula
1)	ACETON	-2.4799E+05	58.0804	$C_3H_6O_1$
2)	AKAR1	-1.2272E+05	201.2475	$C_{12}H_{13}N_2O_1$
3)	AKAR2	-1.0669E+05	226.2790	$C_{14}H_{14}N_2O_1$
4)	AKAR3	-1.5272E+05	240.3042	$C_{15}H_{16}N_2O_1$
5)	AKARD	-1.0669E+05	226.2790	$C_{14}H_{14}N_2O_1$
6)	ALC	-2.7790E+05	46.0694	$C_2H_6O_1$
7)	AMYLPH	-9.2425E+05	306.4036	$C_{18}H_{26}O_4$
8)	AN	-3.6556E+05	80.0432	$N_2H_4O_3$
9)	ARP	0.0000E+00	39.9480	AR_1
10)	ARV	-2.4789E+03	39.9480	AR_1
11)	BANITR	-9.9186E+05	261.3498	$BAN_1O_2{}_6$
12)	BAO	-5.4810E+05	153.3394	$BAO_1{}_1$
13)	C	0.0000E+00	12.0110	C_1
14)	CEDAC	-1.3514E+08	24265.0000	$C_{983}H_{1383}O_{692}$
15)	CETAC	-1.5623E+08	28376.0000	$C_{1179}H_{1579}O_{789}$
16)	CRY	-3.3012E+06	209.9413	$NA_3AL_1F_6$

	BLAKE Name	Heat of Formation (J/mol)	Formula Weight	Formula
17)	DBP	-8.4266E+05	278.3496	$C_{16}H_{22}O_{4}$
18)	DECA	-2.3062E+05	138.2522	$C_{10}H_{18}$
19)	DEGDN	-4.3304E+05	196.1172	$C_{4}H_{8}N_{2}O_{7}$
20)	DNT	-7.1546E+04	182.1360	$C_{7}H_{6}O_{4}N_{2}$
21)	DPA	1.3000E+05	169.2267	$C_{12}N_{1}H_{11}$
22)	EC	-1.0502E+05	268.3598	$C_{17}H_{20}O_{1}N_{2}$
23)	EGLY	-4.5493E+05	62.0688	$C_{2}H_{6}O_{2}$
24)	EOAN	-5.1714E+05	124.0962	$C_{2}H_{8}N_{2}O_{4}$
25)	ETHER	-2.7928E+05	74.1234	$C_{4}H_{10}O_{1}$
26)	ETOH	-2.7790E+05	46.0694	$C_{2}H_{6}O_{1}$
27)	H2O	-2.8583E+05	18.0154	$H_{2}O_{1}$
28)	H2P	0.0000E+00	2.0158	H_{2}
29)	H2V	-2.4789E+03	2.0158	H_{2}
30)	HAN	-3.6652E+05	96.0430	$N_{2}H_{4}O_{4}$
31)	HEP	0.0000E+00	4.0026	HE_{1}
32)	HEV	-2.4789E+03	4.0026	HE_{1}
33)	HMX	7.4894E+04	296.1560	$C_{4}H_{8}O_{8}N_{8}$
34)	HNO3	-1.7410E+05	63.0129	$H_{1}N_{1}O_{3}$
35)	IPAN	-4.0334E+05	122.1250	$C_{3}H_{10}O_{3}N_{2}$

	BLAKE Name	Heat of Formation (J/mol)	Formula Weight	Formula
36)	JA2	-2.3559E+09	1034408.1875	C 21039 H 30756 O 37770 N 10435
37)	KN	-4.9271E+05	101.1029	K 1 N 1 O 3
38)	KS	-1.4337E+06	174.2536	K 2 S 1 O 4
39)	MC	-7.3220E+04	240.3058	C 15 H 16 N 2 O 1
40)	METRIO	-4.4350E+05	255.1420	C 5 H 9 N 3 O 9
41)	MGO	-6.0166E+05	252.5066	MG 1 O 1
42)	N2P	0.0000E+00	28.0134	N 2
43)	N2V	-2.4789E+03	28.0134	N 2
44)	NDPA	6.4434E+04	214.2242	C 12 H 10 O 2 N 2
45)	NG	-3.7070E+05	227.0872	C 3 H 5 O 9 N 3
46)	NNDP	2.2594E+04	259.2217	C 12 H 9 O 4 N 3
47)	NQ	-9.2466E+04	104.0686	C 1 H 4 O 2 N 4
48)	O2P	0.0000E+00	31.9988	O 2
49)	O2V	-2.4789E+03	31.9988	O 2
50)	PB2CO4	-9.1839E+05	490.4086	PB 2 C 1 O 4
51)	PBO	-4.3304E+05	223.1994	PB 1 O 1
52)	PETN	-5.3890E+05	316.1386	C 5 H 8 O 12 N 4
53)	RDX	6.6526E+04	222.1176	C 3 H 6 N 6 O 6
54)	TATB	-1.3975E+05	222.1170	C 3 H 6 N 6 O 6

	BLAKE Name	Heat of Formation (J/mol)	Formula Weight	Formula
55)	TEAN	-9.5261E+05	212.2022	C 6 H 16 N 2 O 6
56)	TEGDN	-6.0626E+05	240.1710	C 6 H 12 N 2 O 8
57)	TMAN	-3.1003E+05	122.1246	C 3 H 10 N 2 O 3
58)	TRIAC	-1.1723E+06	218.2070	C 9 H 14 O 6
59)	WATER	-2.8583E+05	18.0154	H 2 O 1
60)	XM46	-5.1355E+09	1842482.2500	N 11694 H 50100 O 33821 C 4385
61)	JA2	-2.3559E+09	1034155.6480	C 21039 H 30756 O 37770 N 10435
62)	NC1111	-7.5358E+08	252132.4063	C 6000 H 8000 O 9000 N 2000
63)	NC1112	-7.5333E+08	252258.4063	C 6000 H 7997 O 9005 N 2003
64)	NC1113	-7.5304E+08	252384.5938	C 6000 H 7995 O 9011 N 2005
65)	NC1114	-7.5274E+08	252510.9063	C 6000 H 7992 O 9017 N 2008
66)	NC1115	-7.5245E+08	252637.2031	C 6000 H 7989 O 9022 N 2011
67)	NC1116	-7.5216E+08	252763.7969	C 6000 H 7986 O 9028 N 2014
68)	NC1117	-7.5187E+08	252890.4063	C 6000 H 7983 O 9033 N 2017
69)	NC1118	-7.5161E+08	253017.2031	C 6000 H 7980 O 9039 N 2020
70)	NC1119	-7.5132E+08	253144.0938	C 6000 H 7978 O 9045 N 2022
71)	NC1120	-7.5103E+08	253271.0938	C 6000 H 7975 O 9050 N 2025
72)	NC1121	-7.5074E+08	253398.2969	C 6000 H 7972 O 9056 N 2028
73)	NC1122	-7.5044E+08	253525.5938	C 6000 H 7969 O 9062 N 2031

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Appendix D.

INPUT FOR THE SAMPLE CASES

This is a listing of the 9 sample cases referred to in Sec. IX. The outputs they generate are listed in full in Appendix E.

```
TITle, CASE 1: The FORmula, COMposition, and GUN instructions
FORmula, AN, -8.7370E+04, N, 2, O, 3, H, 4, C
COMposition, AN, 75
GUN, 0.05, 0.05, 0.40
STOP

TITle, CASE 2: The MORe, BPR, and UNIts instructions
PRL, CON, 0
MORe,1
BPR,1
UNIts, ENG
COMposition, NC1326,85,NG,15, CRY, 3
GUN, .05, .05, 0.20
STOP

TITle, CASE 3a: An unsuccessful black powder calculation
FOR,ROSEB,-74.53E6,C,8681,H,4962,S,1.2,N,27,O,1000, C
For, S, 0, S, 1
Prl, Con, 2
Time, 1
COM, KN, 73.88, S, 9.97, H2O, 1, ROSEB, 15.71
GUN, 1E-4, 1E-4,5.9E-4
GUN, 0.0006, 1E-4, 0.0021
GUN, .0022, 1E-4, .0038
GUN, .0039, 1E-4, .0049
GUN, .05, .05,.4
STOP

TITle, CASE 3b: A successful black powder calculation
FOR,ROSEB,-74.53E6,C,8681,H,4962,S,1.2,N,27,O,1000, C
For, S, 0, S, 1
PRL,CON,0
REJ,   KOH$,  C(S)
RET
TIM, 5
COM, KN, 73.88, S, 9.97, H2O, 1, ROSEB, 15.71
GUN, 1E-4, 1E-4, 6E-4
GUN, 0.0007, 1E-4, 0.0022
GUN, .0023, 1E-4, .0039
GUN, .0040, 1E-4, .0050
GUN, .006, 0.001, 0.019
GUN, .02, 0.01, 0.17
GUN, 0.18, 0.01, 0.20
GUN, 0.25, 0.05, 0.40
STOP
```

```
TITle, CASE 3c: A better black powder calculation
FOR,ROSEB,-74.53E6,C,8681,H,4962,S,1.2,N,27,O,1000, C
FOR, S, 0, S, 1
REJ, KOH$, C(S)
RET
COM, KN, 73.88, S, 9.97, H2O, 1, ROSEB, 15.71
   Reverse order of loading densities (suggested by P. Baer)
GUN, 0.00059, -0.0001, 0.0001
STOP

TITle, CASE 4: The closed-BOMb instruction (BOMb)
PRL, CON, 0
COMposition, NC1326,85,NG,15, CRY, 3
BOMb, V, 500, W, 100
STOP

TITle, CASE 5: A GUN calculation, followed by an isentropic expansion
PRL, CON, 0
COMposition, NC1326,85,NG,15,
    A GUN instruction is needed to determine the initial
    entropy.
GUN, .2, 10, 0
   Now run an ISOline instruction.
    Note that no numerical value for S has to be input.
ISOline, S, , V, 5, 3, 100
STOP

TITle, CASE 6: A POInt calculation--constant pressure flame
    First run a COMposition instruction to determine H(0)
PRL, CON, 0
COMposition, NC1326,85,NG,15,
    Now run the POInt instruction
POInt, p, 0.101325, h, -2306.1
STOP

TITle, CASE 7: Electrothermal GUN calculation with 2 libraries.
INGRED
PRL, CON, 0
COMposition, JA2, 1
GUN, .2, 10, 0, 10
LIB, X
COMposition, JA2, 1
GUN, .2, 10, 0, 10
STOp

TITle, CASE 8: A heat of explosion calculation
PRL, CON, 0
COM, nc1316, 85, dbp, 15
QEXplosion, R, , T, 1500, 4,    P
STOp
```

```
Title, CASE 9: Forming a plot file
PRL, CON, 0
     ONE = M1A1, a single base propellant
     TWO = M30A1, a triple base propellant
   THREE = a double base propllant
For, ONE, -2.349E+09, C, 21019, H, 30726, O, 37803, N, 10453,
For, TWO, -4.518E+09, C, 19742, H, 20221, O, 40219, N, 11498,
For, THREE, -2.287E+06,  C, 20.004, H, 27.296, O, 40.817, N, 11.883
plot
tit, ONE / TWO / THREE = 1 / 0 / 0
com, one, 1, two, 0, three, 0
gun, 0.01, 0.01, 0.32

Tit, ONE / TWO = 90 / 10
Com, one, 9, two, 1
gun, .2, 10, 0
tit, ONE / TWO / THREE = 90 /  5 /  5
com, one, 90, two,  5, three,  5
gun, .2, 10, 0
tit, ONE / TWO / THREE = 80 / 10 / 10
com, one, 80, two, 10, three, 10
gun, .2, 10, 0
tit, ONE / TWO / THREE = 50 / 25 / 25
com, one, 50, two, 25, three, 25
gun, .2, 10, 0
tit, ONE / TWO / THREE = 10 / 50 / 40
com, one, 10, two, 50, three, 40
gun, .2, 10, 0
stop
```

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Appendix E.

OUTPUT FROM THE SAMPLE CASES

The output for Case 1:

```
************  BLAKE Thermodynamic Equilibrium & Gun Code  ******************
*           ARLware < Director, WMRD/ARL, APG, MD  21005-5066                *
*                     Attn : A. Kotlar, AMSRL-WM-BD >                        *
*****************************************************************************

                        ***  BLAKE   Version 221.4  ***

          Tyger! Tyger! Burning bright/ In the forests of the night.
          What immortal hand or eye/ Dare frame thy fearful symmetry?
                                      ---William Blake  (1757-1827)

      16:11:11                                                  14-APR-1998

> TITle, CASE 1: The FORmula, COMposition, and GUN instructions

> FORmula, AN, -8.7370E+04, N, 2, O, 3, H, 4, C

Duplicate FORmula Name -- Be CAREFUL!
FORmula, AN, -8.7370E+04, N, 2, O, 3, H, 4, C


> COMposition, AN, 75

    ********************************************************************
    <<<          The binary library being used is based on            >>>
    <<<                SBLAKLYB.LIB dated 27 NOV 1997                 >>>
    <<<                                                               >>>
    <<<        This binary library was created on 28-MAR-1998         >>>
    ********************************************************************



      16:11:11                                  14-APR-1998  Page  1.

        CASE 1: The FORmula, COMposition, and GUN instructions

                              THE COMPOSITION IS

  Name      Pct Wt     Pct Mole     Delta H (J/mol)          FORMULA

     AN   100.000     100.000        -3.6556E+05       N      O      H
                                                         2      3      4

The Elements and their Atom Percentages
```

N	22.222
O	33.333
H	44.444

Formula Weight = 889.356

The Heat of Formation is -4567.0 J/g = -4.062E+06 J/mol
=-1091.56 cal/g = -9.708E+05 cal/mol

> GUN, 0.05, 0.05, 0.40

CONSTITUENT CONCENTRATIONS - MOLES PER KGM OF COMPOUND

NAME		1)	2)	3)	4)
H2O	GAS	2.49847E+01	2.49851E+01	2.49832E+01	2.49835E+01
N2	GAS	1.24722E+01	1.24703E+01	1.24677E+01	1.24658E+01
O2	GAS	6.22359E+00	6.22105E+00	6.21797E+00	6.21536E+00
OH	GAS	3.02910E-03	2.64087E-03	2.46911E-03	2.37362E-03
H2	GAS	1.55918E-05	1.15998E-05	9.93897E-06	9.01319E-06
O	GAS	8.94103E-06	6.98598E-06	6.27625E-06	5.95838E-06
H	GAS	5.50941E-08	3.61635E-08	2.93003E-08	2.58127E-08
NH3	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
NO	GAS	3.93545E-02	4.20437E-02	4.48678E-02	4.78436E-02
NH2	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
NH	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
HNO	GAS	1.48200E-07	2.01243E-07	2.53708E-07	3.10000E-07
HO2	GAS	9.55670E-05	1.21694E-04	1.44020E-04	1.65345E-04
N	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
N2O	GAS	2.21801E-05	3.54196E-05	4.89692E-05	6.38318E-05
HNO2	GAS	1.41976E-04	2.58143E-04	3.78535E-04	5.08663E-04
NO2	GAS	2.37534E-03	3.63153E-03	4.80896E-03	6.00647E-03
TOTAL GAS (MOLES/KG)		43.7256	43.7252	43.7216	43.7216

CONSTITUENT CONCENTRATIONS - MOLES PER KGM OF COMPOUND

NAME		5)	6)	7)	8)
H2O	GAS	2.49836E+01	2.49837E+01	2.49841E+01	2.49848E+01
N2	GAS	1.24636E+01	1.24612E+01	1.24587E+01	1.24557E+01
O2	GAS	6.21249E+00	6.20941E+00	6.20611E+00	6.20245E+00
OH	GAS	2.31514E-03	2.27774E-03	2.25348E-03	2.23784E-03
H2	GAS	8.42414E-06	8.02022E-06	7.72967E-06	7.51357E-06
O	GAS	5.82081E-06	5.78344E-06	5.80835E-06	5.87482E-06
H	GAS	2.37617E-08	2.24582E-08	2.15915E-08	2.09996E-08
NH3	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
NO	GAS	5.09738E-02	5.42667E-02	5.77306E-02	6.13739E-02
NH2	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
NH	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
HNO	GAS	3.72031E-07	4.41179E-07	5.18664E-07	6.05719E-07
HO2	GAS	1.86603E-04	2.08262E-04	2.30602E-04	2.53821E-04
N	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
N2O	GAS	8.05579E-05	9.96107E-05	1.21449E-04	1.46571E-04
HNO2	GAS	6.51779E-04	8.10672E-04	9.88065E-04	1.18686E-03
NO2	GAS	7.26598E-03	8.61453E-03	1.00736E-02	1.16628E-02
TOTAL GAS (MOLES/KG)		43.7211	43.7207	43.7203	43.7198

```
                * * SUMMARY OF PROPELLANT THERMO PROPERTIES * *

 Truncated virial equation of state with L-J 6,12 potential is being used

   Rho/L    Temp    Press   Imptus  Mol Wt Co-Vol  Frozen  Balrgy    U      PHI
    g/cc     K       MPa     J/g      Gas   cc/g    Gamma   J/g     J/g
 1).05000  1565.   29.33    569.1  22.870  .595   1.2579  2207.1 -4567.0 1.0307
 2).10000  1578.   61.12    573.6  22.870  .615   1.2706  2120.0 -4567.0 1.0655
 3).15000  1590.   95.76    578.0  22.872  .631   1.2820  2049.5 -4567.0 1.1046
 4).20000  1602.   133.7    582.3  22.872  .644   1.2924  1991.9 -4567.0 1.1477
 5).25000  1614.   175.3    586.7  22.872  .653   1.3018  1943.7 -4567.0 1.1950
 6).30000  1626.   221.0    590.9  22.872  .659   1.3106  1902.7 -4567.0 1.2465
 7).35000  1637.   271.2    595.2  22.873  .663   1.3188  1866.9 -4567.0 1.3020
 8).40000  1649.   326.4    599.4  22.873  .664   1.3266  1834.9 -4567.0 1.3616

> STOP

Run time =     2.09 seconds
```

The output for Case 2:

```
************  BLAKE Thermodynamic Equilibrium & Gun Code  ******************
*           ARLware < Director, WMRD/ARL, APG, MD  21005-5066                *
*                     Attn : A. Kotlar, AMSRL-WM-BD >                        *
*************************************************************************

                        ***  BLAKE   Version 221.4  ***

          Tyger! Tyger! Burning bright/ In the forests of the night.
          What immortal hand or eye/ Dare frame thy fearful symmetry?
                                      ---William Blake  (1757-1827)

      16:11:15                                                 14-APR-1998

> TITle, CASE 2: The MORe, BPR, and UNIts instructions

> PRL, CON, 0

> MORe,1

> BPR,1

> UNIts, ENG

> COMposition, NC1326,85,NG,15, CRY, 3

    ****************************************************************
    <<<         The binary library being used is based on          >>>
    <<<               SBLAKLYB.LIB dated 27 NOV 1997               >>>
    <<<                                                            >>>
    <<<       This binary library was created on 28-MAR-1998       >>>
    ****************************************************************
```

CASE 2: The MORe, BPR, and UNIts instructions

THE COMPOSITION IS

Name	Pct Wt	Pct Mole	Delta H (J/mol)	FORMULA
NC1326	82.524	.374	-6.8500E+08	C 6000 H 7326 O 10348 N 2674
NG	14.563	82.112	-3.7090E+05	C 3 H 5 O 9 N 3
CRY	2.913	17.514	-3.3012E+06	NA 3 AL 1 F 6

The Elements and their Atom Percentages

C	21.337
H	26.993
O	39.491
N	10.679
NA	.450
AL	.150
F	.900

Formula Weight = 1096.370

The Heat of Formation is -2690.6 J/g = -2.950E+06 J/mol
= -643.09 cal/g = -7.051E+05 cal/mol

> GUN, .05, .05, 0.20

* * SUMMARY OF PROPELLANT THERMO PROPERTIES * *

Truncated virial equation of state with L-J 6,12 potential is being used

	Rho/L g/cc	Temp K	Press MPa	Imptus J/g	Mol Wt Gas	Co-Vol cc/g	Frozen Gamma	Balrgy J/g	U J/g	PHI
1)	.05000	3384.	55.65	1056.6	26.628	1.014	1.2165	4881.3	-2690.6	1.0534
2)	.10000	3416.	118.2	1064.1	26.692	.996	1.2164	4916.5	-2690.6	1.1106
3)	.15000	3433.	187.7	1068.0	26.728	.977	1.2172	4916.2	-2690.6	1.1718
4)	.20000	3445.	264.9	1070.8	26.750	.958	1.2187	4896.8	-2690.6	1.2370

	Rho/L g/cc	Temp K	Press MPa	Cp(Frz) J/Mol-K	B(T) cc	C(T) cm**6	S J/g-K	Gas Vol cc/g	AdExp
1)	.0500	3384.	55.6	46.97	27.3	594.7	9.36	20.00	1.249
2)	.1000	3416.	118.2	47.27	27.3	594.5	9.13	10.00	1.323
3)	.1500	3433.	187.7	47.51	27.3	594.2	8.99	6.67	1.395
4)	.2000	3445.	264.9	47.74	27.3	594.0	8.89	5.00	1.468

```
          Rho/L   Temp   Pressure   Impetus   Mol Wt   Co-Vol
          g/cc     R       psi      ft-lb/lb  Gas      cu in
     1)   .0500   6091.    8071.    353464.  26.628    28.06
     2)   .1000   6149.   17141.    356005.  26.692    27.56
     3)   .1500   6180.   27227.    357303.  26.728    27.05
     4)   .2000   6201.   38422.    358215.  26.750    26.52

> STOP
```

The VIRIALS file for this case:

```
              CASE 2: The MORe, BPR, and UNIts instructions
       T =      3445.    B(T) =   27.290    C(T) =  594.041
   CO2:  37.0     N2:  34.2     CO:  33.0    H2O:  22.3     H2:  22.3
   CH4:  34.3    NH3:  23.3    HCN:  28.7   CH2O:  30.6     NO:  30.7
   CH3:  30.6   C2H2:  30.6   C2H4:  40.3 FORMAC:  30.6      H:  30.6
   CHO:  30.6

Run time =      3.46 seconds
```

The output for Case 3a:

```
************  BLAKE Thermodynamic Equilibrium & Gun Code  ******************
*           ARLware < Director, WMRD/ARL, APG, MD  21005-5066                *
*                     Attn : A. Kotlar, AMSRL-WM-BD >                        *
*****************************************************************************

                        ***  BLAKE   Version 221.4  ***

          Tyger! Tyger! Burning bright/ In the forests of the night.
          What immortal hand or eye/ Dare frame thy fearful symmetry?
                                      ---William Blake  (1757-1827)

      16:11:20                                                  14-APR-1998

> TITle, CASE 3a: An unsuccessful black powder calculation

> For,ROSEB,-74.53E6,C,8681,H,4962,S,1.2,N,27,O,1000, C

> For, S, 0, S, 1

> Prl, Con, 2

> Time, 1

> COM, KN, 73.88, S, 9.97, H2O, 1, ROSEB, 15.71

    ****************************************************************
    <<<         The binary library being used is based on          >>>
    <<<               SBLAKLYB.LIB dated 27 NOV 1997               >>>
    <<<                                                            >>>
    <<<       This binary library was created on 28-MAR-1998       >>>
    ****************************************************************
```

CASE 3a: An unsuccessful black powder calculation

THE COMPOSITION IS

Name	Pct Wt	Pct Mole	Delta H (J/mol)	FORMULA
KN	73.469	66.590	-4.9463E+05	K 1 N 1 O 3
S	9.914	28.340	0.0000E+00	S 1
H2O	.994	5.059	-2.8583E+05	H 2 O 1
ROSEB	15.623	.011	-3.1183E+08	C 8681 H 4962 S 1 N 27 O 1000

The Elements and their Atom Percentages

K	12.250
N	12.307
O	39.777
S	5.216
H	12.259
C	18.191

Formula Weight = 1685.832

The Heat of Formation is -4139.6 J/g = -6.979E+06 J/mol
= -989.41 cal/g = -1.668E+06 cal/mol

THERE ARE 49 GASEOUS CONSTITUENTS SELECTED

	NAME	BKW CO-VOL	L-J EPS/K	L-J SIGMA	THERMO CONSTANTS A1	A2	A3	A4	A5	A6	A7	A8	A9
1.	CO	390.0	91.7	3.690	5.87089	-.43129	.07317	-.00449	-2.15174	.71602	-.08169	-31173.5	53.2279
2.	H2O	250.0	542.5	2.790	5.56675	1.22142	-.25754	.01882	-2.45805	1.03298	-.13916	-61781.2	49.5032
3.	H2	180.0	59.7	2.827	2.86532	.85371	-.13033	.00829	-.09791	.18582	-.03732	-1184.9	38.1212
4.	N2	148.0	71.4	3.798	5.63953	-.28845	.03901	-.00176	-2.10637	.74173	-.08842	-4426.6	51.5669
5.	CO2	600.0	195.2	3.941	9.22908	-.47367	.07405	-.00362	-2.89116	.65789	-.06182	-102740.4	60.1055
6.	OH	226.0	100.0	3.500	3.38079	.75885	-.15238	.01112	-.60605	.36806	-.05570	7623.8	50.2838
7.	H	13.4	100.0	3.500	2.49997	.00000	.00000	.00000	.00000	.00000	.00000	50621.8	33.4298
8.	NH3	476.0	558.3	2.900	8.92020	1.54165	-.37492	.02678	-4.68843	1.58031	-.18864	-19235.1	48.3452
9.	HCN	359.0	344.7	3.339	8.56713	-.02567	-.01526	.00147	-3.45513	1.11918	-.13917	24821.4	54.8595
10.	CH4	528.0	148.6	3.758	17.46433	-.78762	.04597	.00077	-11.09190	3.40776	-.37359	-36310.6	41.8006
11.	O2	350.0	106.7	3.467	3.87495	.44435	-.05976	.00425	.07886	-.20697	.04245	-3049.4	57.3651
12.	O	212.8	100.0	3.500	2.81809	-.19148	.04764	-.00309	-.24226	.09992	-.01172	57852.6	44.5895
13.	CS	.0	100.0	3.500	4.47918	.19765	-.08223	.01139	-.26645	-.08663	.02449	63385.6	58.8531
14.	KOH	.0	100.0	3.500	6.44313	.67747	-.14425	.01035	-.61541	.27703	-.04915	-59657.6	69.3682
15.	H2S	.0	301.1	3.623	9.31626	-.46685	.06203	-.00264	-4.86753	1.67627	-.20158	-13166.0	53.1080

16.	K	.0	100.0	3.500	6.40224	-2.30615	.55547	-.03066	-3.00604	1.03245	-.12736	15901.2	43.3579
17.	COS	.0	336.0	4.130	8.92854	-.39307	.07527	-.00458	-2.15883	.44845	-.04323	-41022.6	66.5903
18.	SH	.0	100.0	3.500	5.23095	-.03798	-.00791	.00181	-1.95374	.82981	-.10876	29820.9	52.8942
19.	NO	386.0	116.7	3.492	5.76895	-.41099	.07127	-.00443	-1.83474	.55041	-.05568	16831.0	57.0149
20.	CHO	700.0	100.0	3.500	9.48734	-.80401	.14016	-.00881	-4.07803	1.16013	-.11855	1447.9	59.7959
21.	CH2O	.0	100.0	3.500	14.06570	-1.12224	.15319	-.00816	-7.54066	2.13185	-.21686	-42286.2	54.9570
22.	HNCO	.0	100.0	3.500	11.01098	-.00992	-.03459	.00368	-3.68594	.95459	-.10522	-34500.1	66.8992
23.	NH2	.0	100.0	3.500	6.68132	.37825	.02679	-.00827	-2.82616	.99834	-.11958	40028.6	51.7109
24.	CH3	525.0	100.0	3.500	11.24174	.24885	-.11597	.01049	-6.04905	2.03246	-.24498	24400.8	49.5823
25.	NH	.0	100.0	3.500	4.61150	.15474	-.01413	.00190	-1.54825	.65690	-.08891	86915.6	49.1212
26.	C2H2	.0	100.0	3.500	11.18933	.46653	-.10777	.00914	-4.62590	1.49609	-.19448	44194.4	55.7013
27.	HNO	.0	100.0	3.500	8.76599	-.45921	.05879	-.00293	-3.45465	.95661	-.09661	15634.0	59.3539
28.	HO2	.0	100.0	3.500	3.49984	2.11986	-.39144	.02386	.95564	-.58326	.09163	180.3	64.0912
29.	C2H4	372.0	224.7	4.163	19.87107	-.54541	.00268	.00359	-10.53087	2.81388	-.28888	-8984.5	54.5731
30.	N	148.0	100.0	3.500	3.21890	-.37868	.07460	-.00211	-.59433	.21336	-.02708	110789.0	42.3450
31.	CN	.0	100.0	3.500	2.35951	.99255	-.05801	-.00423	1.22130	-.60683	.09524	102472.4	57.2608
32.	N2O	.0	100.0	3.500	9.30400	-.59102	.09360	-.00567	-2.76197	.61433	-.05668	10966.9	62.3288
33.	NCO	.0	100.0	3.500	9.34247	-.63446	.10016	-.00545	-2.57117	.51882	-.04128	29432.2	65.9401
34.	HNO2	.0	100.0	3.500	10.68498	.03031	-.03209	.00310	-2.84959	.55020	-.04737	-28888.1	71.2284
35.	CH2	.0	100.0	3.500	9.45937	-.50498	.05787	-.00265	-5.12780	1.84870	-.23208	84185.2	50.0790
36.	C	.0	100.0	3.500	2.34693	-.01142	.03771	-.00412	.20445	-.08872	.01255	169938.6	44.1189
37.	NO2	.0	100.0	3.500	8.79936	-.66668	.11548	-.00747	-2.33097	.36944	-.01320	-537.5	67.1789
38.	CS2	.0	100.0	3.500	8.36954	-.22762	.05309	-.00346	-1.14470	.07479	.00490	20810.8	70.4643
39.	K2	.0	100.0	3.500	1.67516	-.48290	.17432	-.01521	4.96504	-2.35730	.34190	28658.0	79.2658
40.	NS	.0	100.0	3.500	4.97156	-.15303	.03272	-.00216	-.56839	.04212	.00873	59078.8	62.0242
41.	KO	.0	100.0	3.500	4.49599	.11550	-.00022	.00001	.00599	-.02572	.00176	14188.6	67.4299
42.	S	.0	100.0	3.500	1.84808	.23535	-.00819	-.00138	.65688	-.16695	.01608	65730.8	47.3314
43.	K2H2O2	.0	100.0	3.500	15.63333	.68126	-.16732	.01262	-3.46679	.68278	-.05526	-170223.8	98.7437
44.	SO2	.0	100.0	3.500	7.94300	-.28053	.06208	-.00403	-1.17959	-.02368	.03064	-78281.5	71.2255
45.	SO	.0	100.0	3.500	2.36045	1.26386	-.23833	.01682	1.51999	-.69825	.09743	-218.9	62.7558
46.	S2	.0	100.0	3.500	3.50765	.89142	-.19120	.01581	.40443	-.14948	.01253	28698.8	63.7944
47.	KH	.0	100.0	3.500	4.67594	.04097	.01306	-.00088	-.19535	-.09296	.01976	25757.2	56.7010
48.	S2O	.0	100.0	3.500	7.39630	-.15748	.02852	-.00190	-.45589	-.14917	.03082	-19615.0	77.7613
49.	FORMAC	.0	100.0	3.500	18.30798	-1.42235	.06055	.01034	-7.74771	1.57974	-.11073	-110541.4	67.5943

THE FLOOR IS AT 18

THERE ARE 5 CONDENSED CONSTITUENTS SELECTED:

N A M E		THERMO CONSTS (LIQUID FIRST, THEN SOLID) FOLLOWED BY CONDENSED EQN OF STATE CONSTS (LIQUID FIRST, THEN SOLID)								
(FRMS IN LIB	PRT)	B1/C1	B2/C2	B3/C3	B4/C4	B5/C5	B6/C6	B7/C7	B8/C8	B9/C9
1. C(S)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
	3.66617E+00	-1.88306E-01	5.61111E-02	-3.74389E-03	-8.98978E-01	-6.96655E-02	3.21230E-02	-4.42368E+03	4.32748E+00	
	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
	4.99259E+00	3.96280E-05	1.19136E-09	-6.37753E-06	1.19250E-10	-3.75578E-15	3.58287E-12	-1.00976E-16	0.00000E+00	
2. KOH$	9.99542E+00	9.87635E-09	-4.33577E-09	7.35178E-10	6.33332E-09	-1.77150E-09	1.89208E-10	-1.04561E+05	4.71295E+01	
	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
	2.80000E+01	7.30000E-03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
3. K2CO3$	4.09470E+02	-2.71062E+02	9.13935E+01	-1.17935E+01	-2.65247E+02	8.11791E+01	-9.18049E+00	-6.89866E+05	8.81916E+01	
	3.45518E+00	1.69713E+01	-2.05901E+00	2.96820E-01	5.91103E+00	-2.09660E+00	2.43436E-01	-2.75449E+05	5.76478E+01	
	7.20000E+01	1.75000E-02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	
	6.04000E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	

```
4.    K2S$  9.83193E+01 -5.52426E+01  1.66681E+01 -1.90235E+00 -6.40521E+01  2.04752E+01 -2.38088E+00 -1.80653E+05  4.39148E+01
       -4.90275E+02  5.40866E+02 -2.65209E+02  4.81588E+01  2.27261E+02 -4.95257E+01  4.11249E+00  4.19575E+05 -3.85477E+02
        5.00000E+01  5.00000E-03  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
        4.50000E+01  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
5.  K2SO4$  1.16213E+02 -6.65007E+01  2.19725E+01 -2.69203E+00 -5.78247E+01  1.44612E+01 -1.35678E+00 -4.54290E+05  1.09852E+02
        1.61046E+01  7.18526E+00  1.42717E+00 -3.09719E-01 -1.12363E+00  2.68327E-01 -2.51233E-02 -3.51797E+05  7.51891E+01
        7.48500E+01  1.75000E-02  4.10000E-06  9.59000E-10  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
        6.53700E+01  8.20000E-03  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00

 > GUN, 1E-4, 1E-4,5.9E-4

 No. of suppressed ERROR #30 messages = 26

   >>>  ERROR #25: Time limit exceeded in ECOMPO.

 Run time =     60.15 seconds
```

The output for Case 3b:

```
 ************  BLAKE Thermodynamic Equilibrium & Gun Code  *****************
 *           ARLware < Director, WMRD/ARL, APG, MD  21005-5066               *
 *                     Attn : A. Kotlar, AMSRL-WM-BD >                       *
 *************************************************************************

                          ***  BLAKE   Version 221.4  ***

           Tyger! Tyger! Burning bright/ In the forests of the night.
           What immortal hand or eye/ Dare frame thy fearful symmetry?
                                      ---William Blake  (1757-1827)

       16:12:21                                                 14-APR-1998

 > TITle, CASE 3b: A successful black powder calculation

 > FOR,ROSEB,-74.53E6,C,8681,H,4962,S,1.2,N,27,O,1000, C

 > For, S, 0, S, 1

 > PRL,CON,0

 > REJ,    KOH$,   C(S)

 > RET

 > TIM, 5

 > COM, KN, 73.88, S, 9.97, H2O, 1, ROSEB, 15.71
    ***************************************************************
    <<<          The binary library being used is based on          >>>
    <<<                SBLAKLYB.LIB dated 27 NOV 1997               >>>
    <<<                                                             >>>
    <<<        This binary library was created on 28-MAR-1998       >>>
    ***************************************************************
```

CASE 3b: A successful black powder calculation

THE COMPOSITION IS

Name	Pct Wt	Pct Mole	Delta H (J/mol)	FORMULA
KN	73.469	66.590	-4.9463E+05	K 1 N 1 O 3
S	9.914	28.340	0.0000E+00	S 1
H2O	.994	5.059	-2.8583E+05	H 2 O 1
ROSEB	15.623	.011	-3.1183E+08	C 8681 H 4962 S 1 N 27 O 1000

The Elements and their Atom Percentages

K	12.250
N	12.307
O	39.777
S	5.216
H	12.259
C	18.191

Formula Weight = 1685.832

The Heat of Formation is -4139.6 J/g = -6.979E+06 J/mol
= -989.41 cal/g = -1.668E+06 cal/mol

> GUN, 1E-4, 1E-4, 6E-4

* * SUMMARY OF PROPELLANT THERMO PROPERTIES * *

Truncated virial equation of state with L-J 6,12 potential is being used

	Rho/L g/cc	Temp K	Press MPa	Imptus J/g	Mol Wt Gas	Co-Vol cc/g	Frozen Gamma	Balrgy J/g	U J/g	PHI
1)	.00010	1211.	.17	176.6	33.094******		1.2194	804.7	-1235.5	1.0000
2)	.00020	1347.	.39	199.0	33.226******		1.2155	923.7	-1185.1	1.0001
3)	.00030	1645.	.08	271.8	35.616	.691	1.2118	1283.3	-4139.6	1.0002
4)	.00040	1665.	.11	273.7	35.482	.706	1.2114	1294.7	-4139.6	1.0002
5)	.00050	1681.	.14	275.2	35.374	.714	1.2112	1303.2	-4139.6	1.0003
6)	.00060	1693.	.17	276.4	35.282	.721	1.2110	1310.0	-4139.6	1.0003

> GUN, 0.0007, 1E-4, 0.0022

* * SUMMARY OF PROPELLANT THERMO PROPERTIES * *

Truncated virial equation of state with L-J 6,12 potential is being used

	Rho/L g/cc	Temp K	Press MPa	Imptus J/g	Mol Wt Gas	Co-Vol cc/g	Frozen Gamma	Balrgy J/g	U J/g	PHI
1)	.00070	1704.	.19	277.3	35.203	.725	1.2108	1315.6	-4139.6	1.0004
2)	.00080	1713.	.22	278.2	35.134	.773	1.2107	1320.3	-4139.6	1.0005
3)	.00090	1721.	.25	278.9	35.071	.756	1.2106	1324.4	-4139.6	1.0005
4)	.00100	1728.	.28	279.5	35.015	.749	1.2105	1328.0	-4139.6	1.0006
5)	.00110	1735.	.31	280.1	34.964	.746	1.2104	1331.1	-4139.6	1.0006
6)	.00120	1740.	.34	280.6	34.917	.744	1.2104	1333.9	-4139.6	1.0007
7)	.00130	1746.	.37	281.1	34.873	.744	1.2103	1336.5	-4139.6	1.0007
8)	.00140	1750.	.39	281.5	34.833	.745	1.2103	1338.8	-4139.6	1.0008
9)	.00150	1755.	.42	281.9	34.795	.745	1.2102	1340.9	-4139.6	1.0009
10)	.00160	1759.	.45	282.3	34.760	.746	1.2102	1342.9	-4139.6	1.0009
11)	.00170	1763.	.48	282.6	34.727	.747	1.2102	1344.7	-4139.6	1.0010
12)	.00180	1767.	.51	282.9	34.695	.748	1.2101	1346.4	-4139.6	1.0010
13)	.00190	1770.	.54	283.2	34.666	.748	1.2101	1347.9	-4139.6	1.0011
14)	.00200	1773.	.57	283.5	34.638	.749	1.2101	1349.4	-4139.6	1.0011
15)	.00210	1776.	.60	283.7	34.611	.750	1.2101	1350.8	-4139.6	1.0012
16)	.00220	1779.	.63	284.0	34.586	.750	1.2100	1352.1	-4139.6	1.0012
17)	.00230	1782.	.65	284.2	34.561	.751	1.2100	1353.3	-4139.6	1.0013

> GUN, .0023, 1E-4, .0039

* * SUMMARY OF PROPELLANT THERMO PROPERTIES * *

Truncated virial equation of state with L-J 6,12 potential is being used

	Rho/L g/cc	Temp K	Press MPa	Imptus J/g	Mol Wt Gas	Co-Vol cc/g	Frozen Gamma	Balrgy J/g	U J/g	PHI
1)	.00230	1782.	.65	284.2	34.561	.751	1.2100	1353.3	-4139.6	1.0013
2)	.00240	1784.	.68	284.4	34.538	.752	1.2100	1354.4	-4139.6	1.0014
3)	.00250	1787.	.71	284.6	34.516	.752	1.2100	1355.5	-4139.6	1.0014
4)	.00260	1789.	.74	284.8	34.495	.753	1.2100	1356.5	-4139.6	1.0015
5)	.00270	1791.	.77	285.0	34.475	.753	1.2100	1357.5	-4139.6	1.0015
6)	.00280	1794.	.80	285.2	34.455	.754	1.2100	1358.4	-4139.6	1.0016
7)	.00290	1796.	.83	285.4	34.436	.754	1.2100	1359.3	-4139.6	1.0016
8)	.00300	1798.	.86	285.6	34.418	.755	1.2099	1360.2	-4139.6	1.0017
9)	.00310	1799.	.89	285.7	34.401	.755	1.2099	1361.0	-4139.6	1.0018
10)	.00320	1801.	.92	285.9	34.384	.756	1.2099	1361.7	-4139.6	1.0018
11)	.00330	1804.	.95	286.0	34.361	.756	1.2099	1362.4	-4139.6	1.0019
12)	.00340	1807.	.98	286.2	34.337	.757	1.2099	1363.1	-4139.6	1.0019
13)	.00350	1809.	1.00	286.3	34.315	.757	1.2100	1363.7	-4139.6	1.0020
14)	.00360	1812.	1.03	286.5	34.293	.758	1.2100	1364.3	-4139.6	1.0020
15)	.00370	1814.	1.06	286.6	34.271	.758	1.2100	1364.9	-4139.6	1.0021
16)	.00380	1817.	1.09	286.7	34.250	.759	1.2100	1365.5	-4139.6	1.0021
17)	.00390	1819.	1.12	286.8	34.230	.759	1.2100	1366.0	-4139.6	1.0022
18)	.00400	1821.	1.15	287.0	34.210	.759	1.2100	1366.5	-4139.6	1.0023

> GUN, .0040, 1E-4, .0050

* * SUMMARY OF PROPELLANT THERMO PROPERTIES * *

Truncated virial equation of state with L-J 6,12 potential is being used

	Rho/L g/cc	Temp K	Press MPa	Imptus J/g	Mol Wt Gas	Co-Vol cc/g	Frozen Gamma	Balrgy J/g	U J/g	PHI
1)	.00400	1821.	1.15	287.0	34.210	.759	1.2100	1366.5	-4139.6	1.0023
2)	.00410	1824.	1.18	287.1	34.191	.760	1.2100	1367.0	-4139.6	1.0023
3)	.00420	1826.	1.21	287.2	34.172	.760	1.2100	1367.4	-4139.6	1.0024
4)	.00430	1828.	1.24	287.3	34.154	.761	1.2100	1367.9	-4139.6	1.0024
5)	.00440	1830.	1.27	287.4	34.136	.761	1.2100	1368.3	-4139.6	1.0025
6)	.00450	1832.	1.30	287.5	34.118	.761	1.2101	1368.7	-4139.6	1.0025
7)	.00460	1834.	1.33	287.6	34.101	.762	1.2101	1369.1	-4139.6	1.0026
8)	.00470	1836.	1.36	287.7	34.084	.762	1.2101	1369.4	-4139.6	1.0026
9)	.00480	1838.	1.39	287.8	34.068	.763	1.2101	1369.8	-4139.6	1.0027
10)	.00490	1839.	1.42	287.9	34.052	.763	1.2101	1370.1	-4139.6	1.0027
11)	.00500	1841.	1.45	287.9	34.036	.763	1.2101	1370.5	-4139.6	1.0028

> GUN, .006, 0.001, 0.019

* * SUMMARY OF PROPELLANT THERMO PROPERTIES * *

Truncated virial equation of state with L-J 6,12 potential is being used

	Rho/L g/cc	Temp K	Press MPa	Imptus J/g	Mol Wt Gas	Co-Vol cc/g	Frozen Gamma	Balrgy J/g	U J/g	PHI
1)	.00600	1857.	1.74	288.7	33.895	.766	1.2102	1373.1	-4139.6	1.0033
2)	.00700	1870.	2.04	289.2	33.777	.769	1.2103	1375.0	-4139.6	1.0039
3)	.00800	1881.	2.33	289.6	33.677	.770	1.2104	1376.2	-4139.6	1.0044
4)	.00900	1891.	2.63	289.9	33.591	.774	1.2105	1377.1	-4139.6	1.0049
5)	.01000	1899.	2.92	290.2	33.516	.775	1.2106	1377.6	-4139.6	1.0055
6)	.01100	1907.	3.22	290.4	33.450	.776	1.2107	1377.9	-4139.6	1.0060
7)	.01200	1913.	3.52	290.6	33.392	.777	1.2108	1378.1	-4139.6	1.0065
8)	.01300	1919.	3.82	290.7	33.340	.778	1.2109	1378.1	-4139.6	1.0071
9)	.01400	1925.	4.12	290.8	33.293	.778	1.2110	1378.0	-4139.6	1.0076
10)	.01500	1930.	4.41	290.9	33.250	.779	1.2111	1377.8	-4139.6	1.0081
11)	.01600	1935.	4.71	290.9	33.212	.780	1.2112	1377.5	-4139.6	1.0087
12)	.01700	1939.	5.01	291.0	33.177	.781	1.2113	1377.2	-4139.6	1.0092
13)	.01800	1943.	5.31	291.0	33.146	.782	1.2114	1376.8	-4139.6	1.0097
14)	.01900	1947.	5.61	291.0	33.117	.782	1.2115	1376.4	-4139.6	1.0102

> GUN, .02, 0.01, 0.17

* * SUMMARY OF PROPELLANT THERMO PROPERTIES * *

Truncated virial equation of state with L-J 6,12 potential is being used

	Rho/L g/cc	Temp K	Press MPa	Imptus J/g	Mol Wt Gas	Co-Vol cc/g	Frozen Gamma	Balrgy J/g	U J/g	PHI
1)	.02000	1950.	5.91	291.1	33.090	.783	1.2115	1376.0	-4139.6	1.0108
2)	.03000	1977.	8.94	290.8	32.919	.788	1.2122	1370.4	-4139.6	1.0160
3)	.04000	1994.	11.99	290.3	32.844	.791	1.2128	1364.0	-4139.6	1.0213
4)	.05000	2006.	15.08	289.6	32.817	.793	1.2134	1357.4	-4139.6	1.0266
5)	.06000	2016.	18.21	288.9	32.817	.796	1.2139	1351.0	-4139.6	1.0319
6)	.07000	2025.	21.37	288.2	32.834	.797	1.2144	1344.7	-4139.6	1.0373
7)	.08000	2032.	24.57	287.5	32.861	.799	1.2148	1338.5	-4139.6	1.0427
8)	.09000	2038.	27.82	286.8	32.895	.800	1.2153	1332.5	-4139.6	1.0482
9)	.10000	2044.	31.11	286.2	32.934	.802	1.2157	1326.6	-4139.6	1.0538
10)	.11000	2049.	34.45	285.5	32.971	.803	1.2161	1320.9	-4139.6	1.0594
11)	.12000	2054.	37.87	285.1	32.953	.805	1.2168	1315.4	-4139.6	1.0651
12)	.13000	2058.	41.35	284.8	32.938	.806	1.2174	1310.0	-4139.6	1.0709
13)	.14000	2063.	44.89	284.4	32.927	.808	1.2179	1304.9	-4139.6	1.0768
14)	.15000	2067.	48.49	284.1	32.917	.809	1.2185	1300.0	-4139.6	1.0828
15)	.16000	2071.	52.16	283.7	32.910	.810	1.2191	1295.2	-4139.6	1.0889
16)	.17000	2075.	55.89	283.4	32.904	.811	1.2196	1290.6	-4139.6	1.0951

> GUN, 0.18, 0.01, 0.20

* * SUMMARY OF PROPELLANT THERMO PROPERTIES * *

Truncated virial equation of state with L-J 6,12 potential is being used

	Rho/L g/cc	Temp K	Press MPa	Imptus J/g	Mol Wt Gas	Co-Vol cc/g	Frozen Gamma	Balrgy J/g	U J/g	PHI
1)	.18000	2078.	59.69	283.2	32.900	.812	1.2202	1286.1	-4139.6	1.1014
2)	.19000	2082.	63.57	282.9	32.897	.813	1.2207	1281.8	-4139.6	1.1077
3)	.20000	2085.	67.51	282.6	32.895	.814	1.2212	1277.6	-4139.6	1.1142

> GUN, 0.25, 0.05, 0.40

* * SUMMARY OF PROPELLANT THERMO PROPERTIES * *

Truncated virial equation of state with L-J 6,12 potential is being used

	Rho/L g/cc	Temp K	Press MPa	Imptus J/g	Mol Wt Gas	Co-Vol cc/g	Frozen Gamma	Balrgy J/g	U J/g	PHI
1)	.25000	2100.	88.44	281.4	32.896	.818	1.2237	1257.9	-4139.6	1.1483
2)	.30000	2113.	111.6	280.6	32.910	.820	1.2262	1240.2	-4139.6	1.1855
3)	.35000	2115.	136.0	278.6	32.943	.809	1.2287	1217.8	-4139.6	1.2248
4)	.40000	2125.	164.7	278.5	32.972	.809	1.2311	1205.1	-4139.6	1.2692

> STOP

Run time = 170.27 seconds

The output for Case 3c:

```
************  BLAKE Thermodynamic Equilibrium & Gun Code  ******************
*           ARLware < Director, WMRD/ARL, APG, MD  21005-5066                *
*                     Attn : A. Kotlar, AMSRL-WM-BD >                        *
*****************************************************************************

                        ***  BLAKE   Version 221.4  ***

          Tyger! Tyger! Burning bright/ In the forests of the night.
          What immortal hand or eye/ Dare frame thy fearful symmetry?
                                        ---William Blake  (1757-1827)

      16:15:13                                                  14-APR-1998

> TITle, CASE 3c: A better black powder calculation

> FOR,ROSEB,-74.53E6,C,8681,H,4962,S,1.2,N,27,O,1000, C

> FOR, S, 0, S, 1

> REJ, KOH$, C(S)

> RET

> COM, KN, 73.88, S, 9.97, H2O, 1, ROSEB, 15.71

    ********************************************************************
    <<<          The binary library being used is based on            >>>
    <<<                SBLAKLYB.LIB dated 27 NOV 1997                 >>>
    <<<                                                               >>>
    <<<       This binary library was created on 28-MAR-1998          >>>
    ********************************************************************


      16:15:13                                  14-APR-1998  Page  1.

              CASE 3c: A better black powder calculation

                          THE COMPOSITION IS

  Name      Pct Wt     Pct Mole     Delta H (J/mol)          FORMULA

    KN     73.469      66.590       -4.9463E+05       K     N     O
                                                        1     1     3

     S      9.914      28.340        0.0000E+00       S
                                                        1

   H2O       .994       5.059       -2.8583E+05       H     O
                                                        2     1
```

ROSEB	15.623	.011	-3.1183E+08	C	H	S	N	O
				8681	4962	1	27	1000

The Elements and their Atom Percentages

K	12.250
N	12.307
O	39.777
S	5.216
H	12.259
C	18.191

Formula Weight = 1685.832

The Heat of Formation is -4139.6 J/g = -6.979E+06 J/mol
= -989.41 cal/g = -1.668E+06 cal/mol

> Reverse order of loading densities (suggested by P. Baer)

> GUN, 0.00059, -0.0001, 0.0001

CONSTITUENT CONCENTRATIONS - MOLES PER KGM OF COMPOUND

NAME		1)	2)	3)	4)
CO2	GAS	7.30133E+00	7.33623E+00	7.37988E+00	7.43760E+00
N2	GAS	3.65009E+00	3.65009E+00	3.65009E+00	3.65009E+00
CO	GAS	3.47760E+00	3.44290E+00	3.39952E+00	3.34216E+00
H2O	GAS	2.49796E+00	2.49041E+00	2.48211E+00	2.47300E+00
KOH	GAS	1.49723E+00	1.51452E+00	1.53353E+00	1.55439E+00
K	GAS	4.62653E-01	4.97406E-01	5.42162E-01	6.03522E-01
H2	GAS	3.50934E-01	3.50194E-01	3.49457E-01	3.48795E-01
H2S	GAS	3.45210E-02	3.42785E-02	3.39428E-02	3.34650E-02
COS	GAS	1.17098E-02	1.15097E-02	1.12456E-02	1.08813E-02
SH	GAS	4.05422E-03	4.05711E-03	4.04439E-03	4.00461E-03
H	GAS	2.82910E-04	2.75194E-04	2.65129E-04	2.51354E-04
OH	GAS	1.04137E-04	9.78171E-05	9.01730E-05	8.05886E-05
NH3	GAS	1.23156E-06	1.04294E-06	8.51519E-07	6.56112E-07
O2	GAS	2.08248E-07	1.91754E-07	1.71864E-07	1.47244E-07
CS	GAS	1.65280E-07	1.48712E-07	1.30005E-07	1.08453E-07
HCN	GAS	8.03726E-08	6.56494E-08	5.11925E-08	3.70678E-08
O	GAS	6.56092E-08	6.03393E-08	5.40020E-08	4.61832E-08
CH4	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
NO	GAS	6.47743E-06	5.91536E-06	5.26191E-06	4.48213E-06
CHO	GAS	6.23598E-08	5.15238E-08	4.06441E-08	2.97569E-08
CH2O	GAS	7.41141E-08	6.07157E-08	4.75302E-08	3.46068E-08
HNCO	GAS	5.91994E-08	4.79741E-08	3.70369E-08	2.64594E-08
NH2	GAS	2.49675E-09	2.04538E-09	1.59676E-09	1.15350E-09
CH3	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
NH	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
C2H2	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
HNO	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
HO2	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
C2H4	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
N	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
CN	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
N2O	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

NCO	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
HNO2	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
CH2	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
C	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
NO2	GAS	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
CS2	GAS	4.42250E-06	4.25331E-06	4.03751E-06	3.75225E-06
K2	GAS	1.04445E-04	1.02995E-04	1.00742E-04	9.71065E-05
NS	GAS	1.37212E-06	1.28276E-06	1.17348E-06	1.03571E-06
KO	GAS	1.14428E-05	1.08207E-05	1.00350E-05	9.00466E-06
S	GAS	2.19777E-04	2.24255E-04	2.28401E-04	2.31656E-04
K2H2O2	GAS	1.57038E-03	1.47022E-03	1.35547E-03	1.21889E-03
SO2	GAS	2.86985E-01	3.04850E-01	3.26565E-01	3.54216E-01
SO	GAS	1.19778E-02	1.23858E-02	1.28272E-02	1.33011E-02
S2	GAS	4.51152E-02	4.90871E-02	5.41187E-02	6.08892E-02
KH	GAS	2.22449E-04	2.12835E-04	2.00940E-04	1.85537E-04
S2O	GAS	1.37183E-03	1.43847E-03	1.51380E-03	1.60050E-03
FORMAC	GAS	3.05760E-07	2.50509E-07	1.96137E-07	1.42843E-07
K2CO3$	SOLID	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
K2CO3$	LIQUID	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
K2S$	SOLID	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
K2S$	LIQUID	2.42229E+00	2.41653E+00	2.40929E+00	2.39959E+00
K2SO4$	SOLID	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
K2SO4$	LIQUID	2.29294E-01	2.09136E-01	1.84618E-01	1.53355E-01
TOTAL GAS (MOLES/KG)		19.6361	19.7018	19.7833	19.8900

CONSTITUENT CONCENTRATIONS - MOLES PER KGM OF COMPOUND

NAME		5)	6)
CO2	GAS	7.52171E+00	7.67374E+00
N2	GAS	3.65010E+00	3.65010E+00
CO	GAS	3.25860E+00	3.10755E+00
H2O	GAS	2.46329E+00	2.45550E+00
KOH	GAS	1.57646E+00	1.59323E+00
K	GAS	6.97213E-01	8.78822E-01
H2	GAS	3.48443E-01	3.49555E-01
H2S	GAS	3.27408E-02	3.14565E-02
COS	GAS	1.03366E-02	9.35662E-03
SH	GAS	3.91058E-03	3.66850E-03
H	GAS	2.30881E-04	1.94408E-04
OH	GAS	6.78235E-05	4.85180E-05
NH3	GAS	4.54443E-07	2.40651E-07
O2	GAS	1.15469E-07	7.09921E-08
CS	GAS	8.27777E-08	5.00021E-08
HCN	GAS	2.33858E-08	1.03720E-08
O	GAS	3.61313E-08	2.21372E-08
CH4	GAS	0.00000E+00	0.00000E+00
NO	GAS	3.51124E-06	2.19483E-06

CHO	GAS	1.89365E-08	8.37452E-09
CH2O	GAS	2.20257E-08	9.94601E-09
HNCO	GAS	1.63612E-08	6.98736E-09
NH2	GAS	7.20445E-10	0.00000E+00
CH3	GAS	0.00000E+00	0.00000E+00
NH	GAS	0.00000E+00	0.00000E+00
C2H2	GAS	0.00000E+00	0.00000E+00
HNO	GAS	0.00000E+00	0.00000E+00
HO2	GAS	0.00000E+00	0.00000E+00
C2H4	GAS	0.00000E+00	0.00000E+00
N	GAS	0.00000E+00	0.00000E+00
CN	GAS	0.00000E+00	0.00000E+00
N2O	GAS	0.00000E+00	0.00000E+00
NCO	GAS	0.00000E+00	0.00000E+00
HNO2	GAS	0.00000E+00	0.00000E+00
CH2	GAS	0.00000E+00	0.00000E+00
C	GAS	0.00000E+00	0.00000E+00
NO2	GAS	0.00000E+00	0.00000E+00
CS2	GAS	3.34998E-06	2.69304E-06
K2	GAS	9.07408E-05	7.71928E-05
NS	GAS	8.52820E-07	5.82243E-07
KO	GAS	7.56717E-06	5.29192E-06
S	GAS	2.32490E-04	2.24850E-04
K2H2O2	GAS	1.04536E-03	7.91003E-04
SO2	GAS	3.92327E-01	4.54692E-01
SO	GAS	1.37883E-02	1.41462E-02
S2	GAS	7.10139E-02	9.02410E-02
KH	GAS	1.64013E-04	1.28644E-04
S2O	GAS	1.70261E-03	1.82398E-03
FORMAC	GAS	9.09563E-08	4.11186E-08
K2CO3$	SOLID	0.00000E+00	0.00000E+00
K2CO3$	LIQUID	0.00000E+00	0.00000E+00
K2S$	SOLID	0.00000E+00	0.00000E+00
K2S$	LIQUID	2.38513E+00	2.35765E+00
K2SO4$	SOLID	0.00000E+00	0.00000E+00
K2SO4$	LIQUID	1.10126E-01	3.87041E-02
TOTAL GAS (MOLES/KG)		20.0435	20.3154

* * SUMMARY OF PROPELLANT THERMO PROPERTIES * *

Truncated virial equation of state with L-J 6,12 potential is being used

Rho/L	Temp	Press	Imptus	Mol Wt	Co-Vol	Frozen	Balrgy	U	PHI
g/cc	K	MPa	J/g	Gas	cc/g	Gamma	J/g	J/g	

```
 1).00059  1692.    .16   276.3  35.291  .720  1.2110  1309.4 -4139.6 1.0003
 2).00049  1679.    .13   275.1  35.384  .713  1.2112  1302.5 -4139.6 1.0003
 3).00039  1663.    .11   273.6  35.494  .704  1.2115  1293.7 -4139.6 1.0002
 4).00029  1642.    .08   271.6  35.631  .692  1.2119  1281.9 -4139.6 1.0002
 5).00019  1613.    .05   268.7  35.814  .734  1.2125  1264.4 -4139.6 1.0001
 6).00009  1560.    .02   263.5  36.096  .611  1.2139  1231.9 -4139.6 1.0001

> STOP

Run time =   138.96 seconds
```

The output for Case 4:

```
************  BLAKE Thermodynamic Equilibrium & Gun Code  ******************
*           ARLware < Director, WMRD/ARL, APG, MD  21005-5066                *
*                     Attn : A. Kotlar, AMSRL-WM-BD >                        *
*****************************************************************************

                        ***  BLAKE   Version 221.4  ***

          Tyger! Tyger! Burning bright/ In the forests of the night.
          What immortal hand or eye/ Dare frame thy fearful symmetry?
                                    ---William Blake  (1757-1827)

      16:17:33                                                14-APR-1998

> TITle, CASE 4: The closed-BOMb instruction (BOMb)

> PRL, CON, 0

> COMposition, NC1326,85,NG,15, CRY, 3



    ****************************************************************
    <<<         The binary library being used is based on           >>>
    <<<               SBLAKLYB.LIB dated 27 NOV 1997                >>>
    <<<                                                             >>>
    <<<       This binary library was created on 28-MAR-1998        >>>
    ****************************************************************



      16:17:34                                  14-APR-1998  Page  1.

              CASE 4: The closed-BOMb instruction (BOMb)

                           THE COMPOSITION IS

  Name      Pct Wt    Pct Mole    Delta H (J/mol)          FORMULA
```

```
 NC1326     82.524        .374        -6.8500E+08      C      H      O      N
                                                      6000   7326  10348   2674

     NG     14.563      82.112        -3.7090E+05      C      H      O      N
                                                         3      5      9      3

    CRY      2.913      17.514        -3.3012E+06     NA     AL      F
                                                         3      1      6

The Elements and their Atom Percentages
          C          21.337
          H          26.993
          O          39.491
          N          10.679
         NA            .450
         AL            .150
          F            .900
                                   Formula Weight =     1096.370

The Heat of Formation is -2690.6 J/g     = -2.950E+06 J/mol
                       = -643.09 cal/g = -7.051E+05 cal/mol

> BOMb, V, 500, W, 100


              * * SUMMARY OF PROPELLANT THERMO PROPERTIES * *


Truncated virial equation of state with L-J 6,12 potential is being used

   Rho/L    Temp    Press   Imptus  Mol Wt Co-Vol  Frozen  Balrgy    U      PHI
    g/cc     K       MPa      J/g     Gas    cc/g    Gamma   J/g     J/g
 1).20000  3445.   264.9    1070.7  26.750   .958  1.2187  4896.7 -2690.6 1.2370

> STOP

Run time =      2.14 seconds
```

The output for Case 5:

```
************  BLAKE Thermodynamic Equilibrium & Gun Code  ******************
*           ARLware < Director, WMRD/ARL, APG, MD  21005-5066                *
*                     Attn : A. Kotlar, AMSRL-WM-BD >                        *
*****************************************************************************

                        ***  BLAKE   Version 221.4  ***

          Tyger! Tyger! Burning bright/ In the forests of the night.
          What immortal hand or eye/ Dare frame thy fearful symmetry?
                                    ---William Blake  (1757-1827)

      16:17:37                                          14-APR-1998
```

```
> TITle, CASE 5: A GUN calculation, followed by an isentropic expansion

> PRL, CON, 0

> COMposition, NC1326,85,NG,15,

    ***********************************************************************
    <<<         The binary library being used is based on            >>>
    <<<               SBLAKLYB.LIB dated 27 NOV 1997                 >>>
    <<<                                                              >>>
    <<<       This binary library was created on 28-MAR-1998         >>>
    ***********************************************************************


     16:17:37                                    14-APR-1998  Page  1.

   CASE 5: A GUN calculation, followed by an isentropic expansion

                          THE COMPOSITION IS

  Name      Pct Wt     Pct Mole     Delta H (J/mol)          FORMULA

 NC1326     85.000        .454        -6.8500E+08       C      H      O      N
                                                        6000   7326  10348   2674

    NG      15.000      99.546        -3.7090E+05       C      H      O      N
                                                           3      5      9      3

The Elements and their Atom Percentages
          C         21.662
          H         27.404
          O         40.092
          N         10.842
                                Formula Weight =    1081.093

The Heat of Formation is -2306.3 J/g     = -2.493E+06 J/mol
                         = -551.22 cal/g = -5.959E+05 cal/mol

> GUN, .2, 10, 0

              * * SUMMARY OF PROPELLANT THERMO PROPERTIES * *

Truncated virial equation of state with L-J 6,12 potential is being used

   Rho/L    Temp    Press   Imptus  Mol Wt Co-Vol  Frozen  Balrgy     U      PHI
    g/cc     K       MPa      J/g     Gas   cc/g    Gamma   J/g      J/g
 1).20000  3603.   282.0   1136.3  26.363   .970  1.2175  5225.2 -2306.3 1.2407

>    Now run an ISOline instruction.
```

```
> ISOline, S, , V, 5, 3, 100

                                ISOLINE

Truncated virial equation of state with L-J 6,12 potential is being used
          P            V            T            H            U            S          Rho
       (MPa)        (cc/g)         (K)        (J/g)        (J/g)      (J/g-K)      (g/cc)
       ------------------------------------------------------------------------------------
                       Cv        Alpha         Beta        AdExp        Sigma        Omega
                     (J/g)                                                (m/s)     (K2/S2)

 1)   .2820E+03      5.000       3603.     -896.44     -2306.27        9.012        .2000
                      1.797       5.281       4.288       1.465           .0         .000

 2)   .7246E+02     13.572       2901.    -2448.01     -3431.45        9.012        .0737
                      1.545       4.827       4.462       1.306       1263.9       1.608

 3)   .2032E+02     36.840       2323.    -3534.31     -4282.86        9.012        .0271
                      1.435       4.552       4.425       1.255       2307.5       2.701

 4)   .5868E+01     99.993       1853.    -4358.16     -4944.93        9.012        .0100
                      1.395       4.438       4.394       1.238       3214.5       3.525

> STOP

Run time =      3.79 seconds
```

The output for Case 6:

```
************  BLAKE Thermodynamic Equilibrium & Gun Code  ******************
*           ARLware < Director, WMRD/ARL, APG, MD  21005-5066                *
*                     Attn : A. Kotlar, AMSRL-WM-BD >                        *
*****************************************************************************

                        ***  BLAKE   Version 221.4  ***

          Tyger! Tyger! Burning bright/ In the forests of the night.
          What immortal hand or eye/ Dare frame thy fearful symmetry?
                                      ---William Blake  (1757-1827)

      16:17:42                                                  14-APR-1998

> TITle, CASE 6: A POInt calculation--constant pressure flame

> PRL, CON, 0

> COMposition, NC1326,85,NG,15,
    ***************************************************************
    <<<         The binary library being used is based on          >>>
    <<<               SBLAKLYB.LIB dated 27 NOV 1997               >>>
    <<<                                                            >>>
    <<<       This binary library was created on 28-MAR-1998       >>>
    ***************************************************************
```

```
      16:17:42                                    14-APR-1998  Page  1.

         CASE 6: A POInt calculation--constant pressure flame

                              THE COMPOSITION IS

  Name      Pct Wt     Pct Mole     Delta H (J/mol)          FORMULA

 NC1326     85.000        .454        -6.8500E+08       C     H     O     N
                                                        6000  7326 10348  2674

     NG     15.000      99.546        -3.7090E+05       C     H     O     N
                                                           3     5     9     3
The Elements and their Atom Percentages
          C          21.662
          H          27.404
          O          40.092
          N          10.842
                                  Formula Weight =    1081.093

The Heat of Formation is -2306.3 J/g     = -2.493E+06 J/mol
                         = -551.22 cal/g = -5.959E+05 cal/mol

> POInt, p, 0.101325, h, -2306.1
                         ***  BLAKE   Version 221.4  ***


      16:17:43                                    14-APR-1998  Page  2.

         CASE 6: A POInt calculation--constant pressure flame

Truncated virial equation of state with L-J 6,12 potential is being used

          P           V          T         H         U          S          Rho
        (MPa)       (cc/g)      (K)      (J/g)     (J/g)     (J/g-K)     (g/cc)
       ------------------------------------------------------------------------
                      Cv       Alpha     Beta      AdExp
                    (J/g)

 1)   .1013E+00  8723.850      2748. -2306.10  -3190.02   11.166     .0001
                    3.723      8.975    8.783     1.136

> STOP

Run time =      1.21 seconds
```

The output for Case 7:

```
************  BLAKE Thermodynamic Equilibrium & Gun Code  *****************
*           ARLware < Director, WMRD/ARL, APG, MD  21005-5066               *
*                     Attn : A. Kotlar, AMSRL-WM-BD >                       *
*************************************************************************
```

*** BLAKE Version 221.4 ***

Tyger! Tyger! Burning bright/ In the forests of the night.
What immortal hand or eye/ Dare frame thy fearful symmetry?
---William Blake (1757-1827)

10:07:59 15-APR-1998

```
> TITle, CASE 7: Electrothermal GUN calculation with 2 libraries.

> INGRED

> For,   CAB,   12510160.0, C,    147., H,    237., O,77., J

> For,   DEP,    -776550.4, C,12., H,14., O, 4., J

> For, DPADP,   -1175285.6, C,12., H,22., O, 4., J

> For,DNTROX,    -277650.2, C, 3., H, 6., N, 2., O, 6., J

> For,   ERL, -110457600.0, C,   5354., H,   6934., O,   1485., N,    353., J

> For,   FOM,  -24183520.0, C,    313., H,    503., O,    184., J

> For,  IPDI,    -466097.6, C,12., H,18., O, 2., N, 2., J

> For,   LEC,    -215894.4, C, 5., H,11., J

> For,  R45M,    -180330.4, C,   7000., H,  11000., O,84., N,92., J

> For, ROSEB, -311708000.0, C,   8681., H,   4962., N,27., O,   1000., J

> For, SEBAC,   -1191185.0, C,18., H, 34., O, 4., J

> For,   TMP,    -744752.0, C, 6., H, 14., O, 3., J

> For,   WAX,   59119920.0, C,   6855., H,  12173., O,    336., J

> For,  H2O2,    -187780.0, H, 2., O, 2., J

> For,  METH,    -238529.8, C, 1., H, 4., O, 1., J

> For,  UDMH,     -53095.0, C, 2., H, 8., N, 2., J

> For,  RFNA,-2713742400.0, N,  16294., H,  15722., O,  46950., J

> For,  DIEP,    -105018.4, C,17., H,20., O, 1., N, 2., J

> For,CUBANE,     541800.0, C, 8., H, 8., J

> For,  TAGN,     -48116.0, C, 1., N, 7., H, 9., O, 3., J

> For,   GAP,   14187944.0, C,    300., H,    509., O,    104., N,    308., J
```

```
> For,  KCRY,   -3358100.0, K, 3.,AL, 1., F, 6., J

> For,  XM46,-5135500000.0, N,  11694., H,  50100., O,  33821., C,   4385., J

> For,    AP,   -295.31E3,  N,      1., H,      4., CL,     1., O,      4.,

> For, ADN, -149.8E3, H, 4, N, 4, O, 4

> FOR,HELP1,-1.7216E+7,C,1842,H,3309,N,2159,O,2689,C

> PRL, CON, 0

> COMposition, JA2, 1

    ********************************************************************
    <<<         The binary library being used is based on            >>>
    <<<               SBLAKLYB.LIB dated 27 NOV 1997                 >>>
    <<<                                                              >>>
    <<<       This binary library was created on 28-MAR-1998         >>>
    ********************************************************************


      10:08:00                                  15-APR-1998  Page  1.

       CASE 7: Electrothermal GUN calculation with 2 libraries.

                              THE COMPOSITION IS

  Name      Pct Wt     Pct Mole     Delta H (J/mol)          FORMULA

    JA2   100.000     100.000        -2.3559E+09       C     H     O     N
                                                      21039 30756 37770 10435

The Elements and their Atom Percentages
          C         21.039
          H         30.756
          O         37.770
          N         10.435
                                  Formula Weight =    1034.141

The Heat of Formation is -2278.1 J/g     = -2.356E+06 J/mol
                         = -544.49 cal/g = -5.631E+05 cal/mol

> GUN, .2, 10, 0, 10

The MODIFIED heat of formation is     7721.9 J/g     =  7.9857E+09 J/mol
                                  =     1845.58 cal/g =  1.9086E+09 cal/mol


              * * SUMMARY OF PROPELLANT THERMO PROPERTIES * *
```

Truncated virial equation of state with L-J 6,12 potential is being used

	Rho/L g/cc	Temp K	Press MPa	Imptus J/g	Mol Wt Gas	Co-Vol cc/g	Frozen Gamma	Balrgy J/g	U J/g	PHI
1)	.20000	6933.	729.1	2821.9	20.428	1.129	1.2528	11162.9	7721.7	1.2918

> LIB, X

C H A N G E O F L I B R A R Y:

```
*****************************************************************
<<<         The binary library being used is based on           >>>
<<<         XBLAKLYB.LIB dated   27 March 1993  (S.T. = 3000)   >>>
<<<                                                             >>>
<<<       This binary library was created on 10-NOV-1997        >>>
*****************************************************  **************
```

> COMposition, JA2, 1

10:08:01 15-APR-1998 Page 2.

CASE 7: Electrothermal GUN calculation with 2 libraries.

THE COMPOSITION IS

Name	Pct Wt	Pct Mole	Delta H (J/mol)	FORMULA			
				C	H	O	N
JA2	100.000	100.000	-2.3559E+09	21039	30756	37770	10435

The Elements and their Atom Percentages

C	21.039
H	30.756
O	37.770
N	10.435

Formula Weight = 1034.141

The Heat of Formation is -2278.1 J/g = -2.356E+06 J/mol
= -544.49 cal/g = -5.631E+05 cal/mol

> GUN, .2, 10, 0, 10

The MODIFIED heat of formation is 7721.9 J/g = 7.9857E+09 J/mol
= 1845.58 cal/g = 1.9086E+09 cal/mol

* * SUMMARY OF PROPELLANT THERMO PROPERTIES * *

Truncated virial equation of state with L-J 6,12 potential is being used

```
   Rho/L    Temp    Press   Imptus  Mol Wt Co-Vol  Frozen  Balrgy    U      PHI
    g/cc     K       MPa     J/g     Gas    cc/g    Gamma   J/g     J/g
 1).20000  6935.   728.0   2818.6  20.457 1.128   1.2499 11279.1  7721.7 1.2915

> STOp

Run time =      4.12 seconds
```

The output for Case 8:

```
************  BLAKE Thermodynamic Equilibrium & Gun Code  ******************
*           ARLware < Director, WMRD/ARL, APG, MD  21005-5066                *
*                     Attn : A. Kotlar, AMSRL-WM-BD >                        *
*****************************************************************************

                        ***  BLAKE   Version 221.4  ***

          Tyger! Tyger! Burning bright/ In the forests of the night.
          What immortal hand or eye/ Dare frame thy fearful symmetry?
                                        ---William Blake  (1757-1827)

      18:04:37                                                14-APR-1998

> TITle, CASE 8: A heat of explosion calculation

> PRL, CON, 0

> COM, nc1316, 85, dbp, 15

    ********************************************************************
    <<<         The binary library being used is based on             >>>
    <<<               SBLAKLYB.LIB dated 27 NOV 1997                  >>>
    <<<                                                               >>>
    <<<       This binary library was created on 28-MAR-1998          >>>
    ********************************************************************


      18:04:37                                  14-APR-1998  Page  1.

                CASE 8: A heat of explosion calculation

                             THE COMPOSITION IS

  Name      Pct Wt     Pct Mole     Delta H (J/mol)          FORMULA

 NC1316     85.000        .558        -6.8856E+08       C     H     O     N
                                                        6000  7361 10278  2639

    DBP     15.000      99.442        -8.4260E+05       C     H     O
                                                          16    22     4
```

```
The Elements and their Atom Percentages
          C         26.214
          H         33.411
          O         32.557
          N          7.817
                                Formula Weight =      978.907

The Heat of Formation is -2537.7 J/g     = -2.484E+06 J/mol
                         = -606.53 cal/g = -5.937E+05 cal/mol

> QEXplosion, R, , T, 1500, 4,    P


                  Loading density (includes solids) =    .2000
                            Gas density (no solid) =    .2017
                          Pressure at temp 1300.00 =     87.57 Mpa
                                                   =    864.20 atm
 HEAT OF EXPLOSION (Rho/L = .2000, T/F = 1300.0) = 4417.8 J/g
                                                   = 1055.9 cal/g
           (Percentage of products accounted for = 80.84)


                  Loading density (includes solids) =    .2000
                            Gas density (no solid) =    .2012
                          Pressure at temp 1400.00 =    103.09 Mpa
                                                   =   1017.44 atm
 HEAT OF EXPLOSION (Rho/L = .2000, T/F = 1400.0) = 4010.7 J/g
                                                   =  958.6 cal/g
           (Percentage of products accounted for = 86.40)


                  Loading density (includes solids) =    .2000
                            Gas density (no solid) =    .2007
                          Pressure at temp 1500.00 =    121.78 Mpa
                                                   =   1201.85 atm
 HEAT OF EXPLOSION (Rho/L = .2000, T/F = 1500.0) = 3576.1 J/g
                                                   =  854.7 cal/g
           (Percentage of products accounted for = 92.31)


                  Loading density (includes solids) =    .2000
                            Gas density (no solid) =    .2002
                          Pressure at temp 1600.00 =    140.32 Mpa
                                                   =   1384.89 atm
 HEAT OF EXPLOSION (Rho/L = .2000, T/F = 1600.0) = 3155.8 J/g
                                                   =  754.3 cal/g
           (Percentage of products accounted for = 97.91)


                  Loading density (includes solids) =    .2000
                            Gas density (no solid) =    .2000
                          Pressure at temp 1700.00 =    159.00 Mpa
                                                   =   1569.18 atm
```

```
 HEAT OF EXPLOSION (Rho/L = .2000, T/F = 1700.0) = 2906.0 J/g
                                                 =  694.6 cal/g
          (Percentage of products accounted for = 99.92)

> STOp

Run time =      3.73 seconds
```

Output for Case 9:

[This output is the PLOT file only].:

.0100	100.0	.0	.0	.0	.0	3288.	11.3	1114.1	24.540	1.071	1.2247	4957.2	-2270.3
.0200	100.0	.0	.0	.0	.0	3329.	23.0	1124.6	24.615	1.064	1.2237	5027.8	-2270.3
.0300	100.0	.0	.0	.0	.0	3351.	35.0	1130.0	24.655	1.059	1.2232	5063.2	-2270.3
.0400	100.0	.0	.0	.0	.0	3365.	47.3	1133.5	24.681	1.055	1.2229	5085.3	-2270.3
.0500	100.0	.0	.0	.0	.0	3375.	60.0	1136.1	24.700	1.051	1.2227	5100.6	-2270.3
.0600	100.0	.0	.0	.0	.0	3383.	72.9	1138.1	24.714	1.047	1.2226	5111.5	-2270.3
.0700	100.0	.0	.0	.0	.0	3389.	86.1	1139.7	24.727	1.044	1.2226	5119.5	-2270.3
.0800	100.0	.0	.0	.0	.0	3395.	99.6	1141.0	24.737	1.040	1.2226	5125.3	-2270.3
.0900	100.0	.0	.0	.0	.0	3399.	113.4	1142.2	24.746	1.036	1.2227	5129.4	-2270.3
.1000	100.0	.0	.0	.0	.0	3403.	127.5	1143.2	24.753	1.032	1.2228	5132.0	-2270.3
.1100	100.0	.0	.0	.0	.0	3407.	141.9	1144.1	24.760	1.029	1.2229	5133.4	-2270.3
.1200	100.0	.0	.0	.0	.0	3410.	156.6	1144.9	24.767	1.025	1.2230	5133.7	-2270.3
.1300	100.0	.0	.0	.0	.0	3413.	171.7	1145.6	24.773	1.021	1.2232	5132.9	-2270.3
.1400	100.0	.0	.0	.0	.0	3416.	187.1	1146.3	24.778	1.017	1.2234	5131.3	-2270.3
.1500	100.0	.0	.0	.0	.0	3418.	202.8	1146.9	24.783	1.013	1.2236	5128.8	-2270.3
.1600	100.0	.0	.0	.0	.0	3421.	218.9	1147.4	24.788	1.009	1.2239	5125.5	-2270.3
.1700	100.0	.0	.0	.0	.0	3423.	235.3	1147.9	24.792	1.005	1.2241	5121.5	-2270.3
.1800	100.0	.0	.0	.0	.0	3425.	252.1	1148.4	24.796	1.001	1.2244	5116.7	-2270.3
.1900	100.0	.0	.0	.0	.0	3427.	269.3	1148.8	24.800	.996	1.2248	5111.2	-2270.3
.2000	100.0	.0	.0	.0	.0	3428.	286.8	1149.3	24.804	.992	1.2251	5105.0	-2270.3
.2100	100.0	.0	.0	.0	.0	3430.	304.6	1149.6	24.808	.988	1.2255	5098.2	-2270.3
.2200	100.0	.0	.0	.0	.0	3432.	322.9	1150.0	24.811	.984	1.2259	5090.7	-2270.3
.2300	100.0	.0	.0	.0	.0	3433.	341.5	1150.4	24.815	.979	1.2263	5082.6	-2270.3
.2400	100.0	.0	.0	.0	.0	3435.	360.5	1150.7	24.818	.975	1.2268	5073.8	-2270.3
.2500	100.0	.0	.0	.0	.0	3436.	380.0	1151.0	24.821	.971	1.2273	5064.5	-2270.3
.2600	100.0	.0	.0	.0	.0	3437.	399.8	1151.3	24.825	.966	1.2278	5054.7	-2270.3
.2700	100.0	.0	.0	.0	.0	3439.	420.0	1151.6	24.828	.962	1.2283	5044.2	-2270.3
.2800	100.0	.0	.0	.0	.0	3440.	440.6	1151.8	24.831	.957	1.2288	5033.2	-2270.3
.2900	100.0	.0	.0	.0	.0	3441.	461.7	1152.1	24.834	.953	1.2294	5021.7	-2270.3
.3000	100.0	.0	.0	.0	.0	3442.	483.2	1152.3	24.837	.949	1.2300	5009.7	-2270.3
.3100	100.0	.0	.0	.0	.0	3443.	505.1	1152.5	24.840	.944	1.2306	4997.2	-2270.3
.3200	100.0	.0	.0	.0	.0	3444.	527.5	1152.7	24.843	.940	1.2313	4984.2	-2270.3
.2000	90.0	10.0	.0	.0	.0	3370.	276.5	1110.4	25.231	.983	1.2239	4958.7	-2468.7
.2000	90.0	5.0	5.0	.0	.0	3424.	282.2	1133.0	25.129	.985	1.2236	5066.5	-2361.1
.2000	80.0	10.0	10.0	.0	.0	3420.	277.7	1116.7	25.462	.979	1.2221	5028.8	-2452.0
.2000	50.0	25.0	25.0	.0	.0	3407.	264.4	1068.3	26.515	.960	1.2172	4919.1	-2724.5
.2000	10.0	50.0	40.0	.0	.0	3333.	241.8	983.2	28.189	.934	1.2102	4677.4	-3195.5

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Appendix F.

ERRATA FOR ARBRL-TR-02411

This is a listing of the known errors in the previous BLAKE Users' Guide.

Page

12: Two lines below Eqn. (12), E_T should be E'_T

13: In Eqn. (17), n_g should be n_j

13: In Eqn. (22), lnP should be $\ln\rho$

33: Eqn. (42) should read MW = 44.9975*X + 162.1430

38: 12 lines from top: 2318201526 should be 2318191526

38: 14 lines from top: 231820. should be 231819.

45: In Eqn. (48), in the last term, 6_7 should be b_7.

45: In Eqn. (49), in the second term, $\frac{b\Theta/2.0}{2}$ should be $b_2\Theta/2.0$.

67: 2 lines from bottom: 2e should be ∂e.

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13. ABSTRACT *(Maximum 200 words)*

BLAKE is a general thermodynamics code for use primarily with IBM-compatible desktop personal computers. This code, which was derived from the original version of SRI's TIGER program, is intended primarily for making calculations on the combustion products from conventional military and electrically-heated gun propellants under chamber conditions (temperatures between 1,500 K and 10,000 K, and pressures up to 700 MPa). An important feature of this code is that it embodies a correction for non-ideal gas effects appropriate to its primary application. This correction is derived from a truncated virial equation of state in which the second virial coefficient is computed using the spherically-symmetric Lennard-Jones 6-12 intermolecular potential. The third virial coefficient is derived from a hard-sphere model.

Another useful feature of the code is that it contains enthalpy data for 60 commonly-used propellant ingredients and some compounded propellants. It also contains enthalpy data for all of the various nitrocelluloses containing from 11.10 to 14.00% nitrogen.

This report is a complete guide to the revised code as of December 1997 including some illustrative examples of its use.

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